School of Chemical and Petroleum Engineering
Department of Chemical Engineering

Water and Wastewater Optimization through Process Integration for Industrial Processes

Reza Parand

This thesis is presented for the Degree of
Doctor of Philosophy
Of
Curtin University

June 2014

Declaration

To the best of my knowledge and belief this thesis contains no material previously published by any other person except where due acknowledgment has been made.

This thesis contains no material which has been accepted for the award of any other degree or diploma in any university.

Signature: ………………………………………….

Date: ………………………...

ABSTRACT

Water management has become a very vital issue for process engineers because of the stringent environmental regulation and the rising cost of water resources due to its rapid depletion. One of the active areas in water management is water integration, where the use of freshwater can be minimized via recycle, regeneration, and reuse. Pinch analysis provides a conceptual approach for water network synthesis. Targeting is the first stage in most pinch analysis techniques to provide a baseline for detailed water network design. Surveying the current studies in this area, not much attention has been paid for removal ratio type regeneration unit targeting. Economical evaluation of regeneration problems is lagged behind and water utilities targeting in threshold problems has not been systematically investigated.

A systematic study of water saving opportunities in process industries is conducted in this research using Water Pinch Analysis as a tool. Water saving potential considering reuse/recycle is firstly investigated and existing targeting and design methods are analysed for the selection of a powerful targeting tool for further studies. It has been found that the Composite Table Algorithm (CTA) is capable of handling multiple pinch and threshold problems which are very specific in water reuse/recycle scheme. It is therefore further extended to target various water operations.

In the proposed Extended Composite Table Algorithm (ECTA), all key parameters in regeneration network with known post-regeneration concentration are considered comprising freshwater, regenerated, and wastewater flow rates together with regeneration and waste water concentrations. Case study shows that ECTA is not restricted by limiting composite curve shape and is able to provide result algebraically as well as graphically with no iterative procedure required. These advantages of ECTA are unique compared to the available targeting methods in regeneration problems.

Since the post regeneration concentration has the dominant influence to the total cost of water network, the assumption of fixed post-regeneration concentration is relaxed through further developed Composite Matrix Algorithm (CMA). CMA addresses the total water regeneration network with specified removal ratio type regenerator. Additionally, economic evaluation is taken into account. From this study, some new insights are captured, such as: pinch point migration and the minimum feasible performance of regeneration unit which can serve the network. It is also concluded that, although higher quality regenerated water leads to more water conservation, it does not essentially guarantee the economic optimality.

For water utility targeting in threshold problem, the introduction of multiple utilities is investigated via case studies under three scenarios (1) the employment of pure fresh water source; (2) the harvest of impure utility below the infeasible threshold pinch point; (3) the utilisation of impure utility with the concentration higher than the infeasible pinch concentration. The study brings forward some new issues such as infeasible threshold pinch point concentration and how to recover the feasibility in infeasible threshold problem. In addition, a new target termed the "threshold maximum permissible" concentration is introduced. The results prove that considering higher quality impure water source provides more room for pure fresh water saving.

LIST OF PUBLICATIONS IN SUPPORT OF THE THESIS

1) Parand, R., Yao, H.M., Tadé, M.O., Pareek, V., 2013. Composite table algorithm - A powerful hybrid pinch targeting method for various problems in water integration. *International Journal Chemical Engineering and Applications*. 4, 224-228.

2) Parand, R., Yao, H.M., Tadé, M.O., Pareek, V., 2013. Targeting water utilities for the threshold problem without waste discharge. *Chemical Engineering Research and Design*. 91, 2569-2578.

3) Parand, R., Yao, H.M., Pareek, V., Tadé, M.O., 2014. Use of pinch concept to optimize the total water regeneration network. *Industrial and Engineering Chemistry Research*. 53, 3222-3235

4) Parand, R., Yao, H.M., Pareek, V., Tadé, M.O., Water network synthesis for petrochemical manufacturing towards zero liquid discharge, *9th world conference of chemical engineering*. August 18-23, 2013.

ACKNOWLEDGMENT

I would like to acknowledge many individuals. The accomplishment of this work would not be possible without their technical and emotional support.

I am particularly thankful to my supervisor, Professor Moses Tadé for all of your support during the last three years, starting my PhD studies. I am indebted to you for your enthusiastic support which encourages me to pursue exploratory research continuously. I have learned a lot from your viewpoint on the quality of my work. I also appreciate the opportunities I have had under your supervision.

I would like to express my gratitude to my co-supervisors, Professor Vishnu Pareek and Dr. Hong-Mei Yao. I appreciate your attention, advice, and support toward my research commitments. I have been truly fortunate to interact with this enthusiastic supervisory panel.

The financial support of my research by the Department of Innovation, Industry, Science, and Research in Australia for International Postgraduate Research Scholarship (IPRS), the Office of Research and Development at Curtin University, Perth, Western Australia for providing Australian Postgraduate Award (APA) and the State Government of Western Australia for providing top up scholarship through the Western Australian Energy Research Alliance (WA:ERA) is gratefully acknowledged.

I am grateful to my mother for her unconditional love and support during my studies overseas. I am indebted to my father, the late Dr. Abbas Parand, to guide me in the direction of seeking knowledge. I am forever obliged to my wife, Fereshteh, for her authentic love and unlimited patience. Finally, I am also grateful to my daughter, Paria, for the joy she brings to my life with her wonderful sense of humour.

There are still so many who deserve my acknowledgment. My sincere apologies to all whose names are not mentioned here but have played a role in my achievements.

TABLE OF CONTENT

LIST OF FIGURES

LIST OF TABLES

NOMENCLATURES

Abbreviations

CMA	Composite Matrix Algorithm
CTA	Composite Table Algorithm
ECTA	Extended Composite Table Algorithm
FF	Fixed Flow rate
FL	Fixed Load
ITPP	Infeasible Threshold Pinch Point
LCC	Limiting Composite Curve
MPT	Mass Problem Table
MRPD	Material Recovery Pinch Diagram
PA	Pinch Analysis
PI	Process Integration
RR	Removal Ratio
SK	Sink
SR	Source
TMP	Threshold Maximum Permissible
WCA	Water Cascade Analysis
WCT	Water Cascade Table

Symbols

C_0	post-regeneration concentration
$C_{0\mathrm{opt}}$	optimum post-regeneration concentration
$C_{0\mathrm{tr}}$	transient post-regeneration concentration
CD	disposal charge
CF	freshwater supply cost
C_{fw}	freshwater contaminant concentration
C_k	concentration level
C_{pfw}	freshwater pinch concentration
C_{pr}	reuse/recycle pinch concentration
C_{preg}	regeneration pinch concentration

CR	regeneration cost
C_{reg}	regeneration concentration
C_{SKj}	process sink concentration
C_{SRi}	of process source concentration
CT	total cost
Cum.Δm	cumulative mass load
C_{ww}	wastewater contaminant concentration
F_c	cumulative flow rate
F_{fw}	freshwater flow rate
F_{ifw}	flow rate of impure fresh water
F_{ifwap}	flow rate of impure fresh water above the pinch
F_{ifwbp}	flow rate of impure fresh water below the pinch
F_{reg}	regenerated water flow rate
F_{SKj}	flow rate of process sink
F_{SRi}	flow rate of process source
F_{ww}	wastewater flow rate
MC_{reg}	regeneration concentration matrix
MF_{reg}	regenerated water flow rate matrix
M_{reg}	regeneration mass load
Δm_k	interval impurity load

1. INTRODUCTION

1.1 Background

Environmental sustainability regulations, the rising cost of raw material and waste treatment, and increasingly stringent emission regulations are the factors that encourage the process industries to use Process Integration (PI) as a promising tool in resource conservation activities to sustain the future human life. (El-Halwagi, 1997, 2006, 2011) defined process integration as a holistic approach to process design, retrofitting, and operation which emphasises the unity of the process.

Water is one of the main resources used by many industries. It is extensively utilised in the processes such as striping, liquid-liquid extraction, and washing operation. Rapid depletion of water resources along with increased water demand causes a water scarcity which severely affects our future generations. Reported by the United Nation (News, 22 March 2002), if water is continued to be consumed at the same rate as it is, by 2025, more than 2.7 billion people will face difficulties to find water**.** Therefore, water conservation activities have attracted the attention of policy makers, researchers, and industrial practitioners. Among these practices, water saving through process integration technology has made a remarkable progress (El-Halwagi, 2011; Foo, 2012; Klemes, 2013; Klemes et al., 2010; Mann and Liu, 1999).

Industrial water network synthesis considering PI is conducted under two popular approaches: insight-based (Water Pinch Analysis (WPA)) and mathematical modelling. Problem dimensionality and computational effectiveness are the advantages of mathematical modelling, especially, when dealing with complex water distribution system involving multiple contaminants. Nevertheless, mathematical modelling is less popular among engineers because it is difficult to formulate the problem model. In addition, designers have less control over the solution space and also have little insights on water network design. On the other hand, methodologies based on WPA are easier to understand, conduct and apply. WPA approaches provide in-depth view and control for the engineers to design the water network. Most of the methods comprise of two subsequent stages known as targeting and design. In the targeting stage the base line for synthesising the water network is set. The main power of WPA methodologies is to identify the potential network for water saving in a relatively simple but meaningful way. However, it remains a challenge for WPA to deal with multiple contaminants problem.

By using WPA, water usage and wastewater generation can be minimized through:

- *Process changes:* The demand for water can be diminished through the substitution of process equipment, e.g., wet cooling towers by dry air coolers.
- *Reuse/recycle:* Wastewater from a water using process is sent to other processes or re-enter the process where it is produced.
- *Regeneration-reuse/recycle:* Wastewater is partially treated by water purification facilities such as filter, stripper, etc., before reuse or recycle in a regeneration scheme.

The successful applications of WPA for network synthesis have been documented in various process industries such as pulp and paper (Tan et al., 2007), petrochemical (Mann and Liu, 1999), food processing (Brouckaert and Buckley, 2000), municipal (Manan et al., 2006), and mineral (Deng and Feng, 2009) to list a few.

1.2 Motivations for this work

The amount of water consumption and in turn wastewater generation has been increasing rapidly in Australia. CSIRO reported that one of the specific objectives in Australia is to reduce average unit water usage and average unit residue production by 20 per cent of 2007 levels by 2025 (CSIRO). To this extent, process integration can be a useful tool for fresh water saving and for the identification of water regeneration-reuse/recycle opportunities. Therefore, developing a framework that can address all water minimization aspects holistically will benefit Australian industries.

However, from the current practice, there are several gaps/unsolved problems/challenges in the application of PI in water network synthesis:

1) The existing application of PI approach in water network synthesis mainly focuses on normal network without considering the opportunities of water saving in specific "threshold problems". These kinds of water network problems are very rare but realistic. Threshold problems fall into three categories i.e. zero discharge network with freshwater feed, no freshwater network with wastewater disposal, and network with no freshwater and zero discharge. These classes can be exclusively addressed through reuse/recycle water network implementation. Due to the insufficient availability of process water sources, regeneration- reuse/recycle solution is not under consideration. However, there is opportunity to save pure freshwater in favour of impure utility, especially for the zero discharge network with freshwater feed. Researchers have not paid enough attentions to this problem.
2) Since the introduction of pinch analysis, many methodologies have been developed and later on extended for targeting. They are more or less tailored techniques, i.e. setup to solve particular problems. A robust targeting method which can handle diverse water network problems in reuse/recycle scheme (both algebraically and graphically) is not available.
3) After implementing mere reuse/recycling configuration, partial wastewater treatment and reuse/recycling again provides more space for freshwater saving. This scheme is known as water regeneration-reuse/recycle. The key parameters in this scheme to be identified are freshwater, regenerated water, and waste water flow rates together with regeneration and wastewater concentrations. In WPA, these parameters are targeted based on two criteria: fixed-post regeneration concentration (C_0), or specified removal ratio (RR). For the former criteria, it is necessary to develop a non-iterative, hybrid graphical and numerical targeting method which can set the targets for global water operation. In regeneration-reuse/recycle scheme considering RR criteria, not much attention has been paid to target the key parameters because of the

complexity of the problem in generic sense. However, design with RR type regenerator is important, so effort is worthy to be made in this extent.

4) In the water network involving regeneration, it has been found that the included regenerator has significant impact on the total cost of the network. The total cost rises even exponentially with the increase of regenerator performance. In most of the previous WPA studies, the post-regeneration concentration is assumed to be fixed, which imposes a limitation on economic evaluation of the water network under synthesis. In addition, a pre-assumed post-regeneration concentration lacks justification and does not guarantee a global optimum target. Therefore, it is more practical to relax this parameter while designing the water network.

With the foregone, consequently, this thesis has made significant contributions in the key areas identified above through the solutions of many of the challenges indicated.

1.3 Research contributions

This project aims to use WPA for various specific water usage problems and to develop a systematic methodology for better network targeting and design. To achieve this, the following studies were conducted:

- The introduction of impure water utility in favour of pure freshwater in threshold problem without waste discharge;
- The extension of existing targeting methods for diverse water network problems;
- The development of non-iterative generic targeting technique to set the key parameters in regeneration-reuse/recycle water network based on fixed post regeneration concentration considering global water operations.
- The proposal of new design methodology to screen the profitability of the regeneration-reuse/recycle water network. Applying this new

method, the targets for removal ratio type regeneration unit is also set before designing the network

The research activities being carried out to target these objectives are explained below in detail.

(1) The threshold problems

In the threshold problems, there is possibility to save pure freshwater water source (most expensive utility) to maximum extend with introduction of impure utilities. However, there has not been much attention for this matter before. To address this issue, a new concept of "Infeasible Threshold Problem" is introduced. Using this new physical insight, different scenarios are proposed for utilities targeting and the recovery of problem feasibility is suggested. Water Cascade Analysis (WCA) is also modified to be capable of targeting multiple utilities for threshold problem without waste discharge. Moreover, a new target named as "Threshold Maximum Permissible" concentration is introduced.

(2) Application of Composite Table Algorithm (CTA) for various problems in reuse/recycle water network

Despite the power of CTA to handle normal reuse/recycle problem in a hybrid manner (both graphical and algebraic), applications of this targeting method for some special cases such as threshold problems and multiple pinch problems were not reported. CTA is enhanced to address these problems.

(3) Targeting methodologies development for total water regeneration network

In the development of targeting, at first, improved pure algebraic methodology, Extended Composite Table Algorithm, is proposed based on the assumption of fixed post-regeneration concentration. Subsequently, this assumption is relaxed through the new targeting approach of Composite Matrix Analysis. Application of these methods is studied later by addressing literature problems. Comparing the results with literature, the accuracy of the methods is also verified.

(4) Targeting for removal ratio and economic evaluation

With the Composite Matrix Algorithm (CMA), work is carried out to target total water regeneration network considering removal ratio type regenerator. Some new valuable insight is reported such as pinch migration, and minimum feasible performance of regeneration unit. Moreover, by setting the cost functions and accommodating vector calculation, the total network is studied by taking the economic considerations into account. It has been revealed that higher regeneration performance leads to more pure freshwater saving, but yet causes higher total investment. The optimization study is conducted via CMA framework to set the optimum scenario.

1.4 Thesis outline

To elucidate the research contributions, the map of research methodology and the referring chapters are depicted as in Figure 1.1.

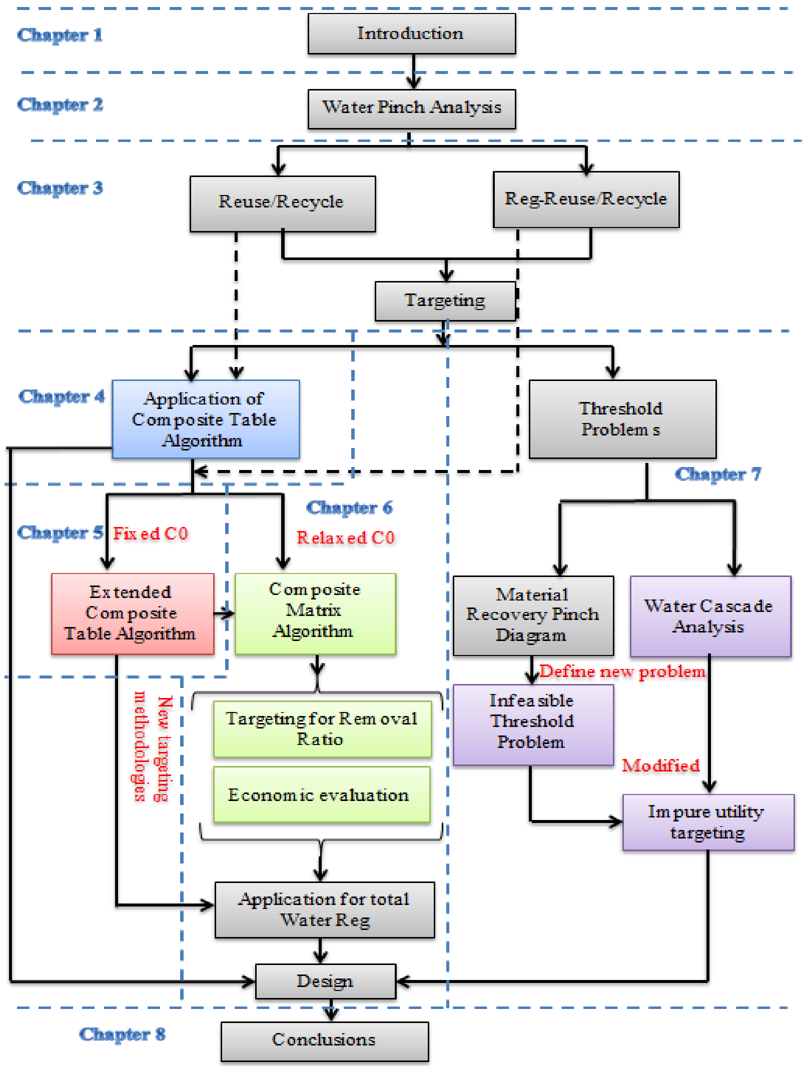

Figure 1.1.Map of research methodology

As shown, the thesis comprises of 8 chapters as follows:

In Chapter 1, some basic information for process integration practices in process industries have been reviewed briefly in background. This chapter also has covered research significance, methodology and specific contribution. The outline of the thesis is also stated.

Literature is reviewed systematically in Chapter 2. The application of process integration in industrial processes is introduced. The basic concept of water network synthesis is elaborated. The techniques in WPA are reviewed, discussed and evaluated. As a result, the limitation of existing techniques is identified. The further studies which are covered in the following chapters are dedicated to address the drawbacks identified in this chapter.

The required background methodologies are provided in Chapter 3. The procedure of four WPA targeting methods known as the Limiting Composite Curve (LCC), Composite Table Algorithm (CTA), Material Recover Pinch Diagram (MRPD), and Water Cascade Analysis (WCA) are elaborated. The two network design methods, Nearest Neighbor Algorithm (NNA), and Tree Design Rules (TDR), are discussed in detail.

In Chapter 4, the capability of CTA to handle various problems addressing reuse/recycle water network is demonstrated. These problems include fixed load, combined fixed load and fixed flow rate, multiple pinch, and threshold problems. The network for each of this problem is then designed. This chapter sets up the foundation for Chapters 5 and 6.

The new targeting methodology for total water regeneration network is proposed in Chapter 5. This method gives both numerical accuracy and conceptual insight for the problem. Furthermore, the application of this method for global water operation is demonstrated. Process flow sheet is also constructed for every case. However, ECTA is developed based on the assumption of specified post-regeneration concentration.

Considering the fact that the post-regeneration concentration has the dominant influence to the total cost of water network, it is relaxed in Chapter 6 through the newly developed method, Composite Matrix Algorithm (CMA). This proposed approach gives an opportunity to set the targets for removal ratio type regenerator and to evaluate the total system on the economic basis. Then the optimum water allocation network is demonstrated.

Chapter 7 is dedicated to the introduction of new insight for water utilities targeting in the threshold problems. The concept of “Infeasible Threshold Problem” is defined via MRPD method. Three different scenarios introduced for utilities targeting leads the feasibility of the problem to be recovered. WCA method is modified and utilised as a complementary approach to MRPD for utilities targeting. The network design for all of scenarios is achieved in practice.

Chapter 8 concludes the thesis with the recommendations and identification of possible future research directions.

Some contributions of this study have been published as journal articles and materials are reused in the thesis with permission from publishers. The details of the publications and their relevant chapters in the thesis are given as follows:

Chapter 4:

Parand, R., Yao, H.M., Tadé, M.O., Pareek, V., 2013. Composite table algorithm - A powerful hybrid pinch targeting method for various problems in water integration. Int. J. Chem. Eng. Appl. 4, 224-228.

Chapters 5 & 6:

Parand, R., Yao, H.M., Pareek, V., Tadé, M.O., 2014. Use of pinch concept to optimize the total water regeneration network. Ind. Eng. Chem. Res. 53, 3222-3235

Chapter 7:

Parand, R., Yao, H.M., Tadé, M.O., Pareek, V., 2013. Targeting water utilities for the threshold problem without waste discharge. Chem. Eng. Res. Des. 91, 2569-2578.

2. LITERATURE REVIEW

In this chapter, some basic information about water network synthesis is provided. Different methodologies in WPA are classified, evaluated and reviewed in detail. The targeting methodologies are categorised under reuse/recycle and regeneration-reuse/recycle problems. Under reuse/recycle scheme, two exclusive problems, multiple utilities, and threshold, are given special attention. The historical development of water pinch targeting methods is clearly mapped. The water network design methodologies are tabulated against their contribution to the problems. These analyses provide an opportunity to find the existing research gaps in the literature and to bridge the gaps systematically through the proposed methodologies in this thesis.

2.1 Water network synthesis in process integration

The term of "process synthesis" was initially introduced by Rudd (Rudd, 1968; Rudd et al., 1973). One of the most comprehensive definitions is described by Westerberg (1987) as : process synthesis is "the discrete decision-making activities of conjecturing (1) which of the many available component parts one should use, and (2) how they should be interconnected to structure the optimal solution to a given design problem". The aim of process synthesis is to determine how each process element is integrated and the flow sheet of design will be obtained to meet pre-specified objectives. Hence, within the process synthesis activity, process inputs (feed streams) and outputs (product streams) are given and it is required either to revise the configuration or parameters of existing flow sheet (retrofit design), or, create a new flow sheet (grass-root design) to cater for certain objectives (El-Halwagi, 1997, 2006). The hierarchical procedure of process synthesis is effectively presented by an onion diagram. In common practice, the reactor (if applicable) is needed before the separation and recycle system to be designed followed by heat recovery system, heating and cooling utilities, water and effluent treatment network design (Douglas, 1985; Smith, 2005). The development of process synthesis from the early establishment can be found in various literature publications (Douglas, 1985, 1992; Dunn and El-Halwagi, 2003;

El-Halwagi and Manousiouthakis, 1989; Gundepsen and Naess, 1988; Hlaváček, 1978; Johns, 2001; Li and Kraslawski, 2004; Manousiouthakis and Allen, 1995; Nishida et al., 1981; Rudd, 1968; Rudd et al., 1973; Smith, 2005; Westerberg, 1987).

Process synthesis, simulation, and optimization are three main elements of comprehensive Process Integration. While the aim of process synthesis is to connect all individual elements together, simulation consists of studying the performance of every element by decomposing them into individuals. Therefore, through simulation, the characteristics (e.g. flow rate, composition, pressure, etc.) of process can be determined after the process has been synthesised. When the process configuration and characteristics has been defined, one should evaluate if this is the best solution. It can be achieved by introducing the process objectives and conducting optimization. Process synthesis and simulation are iteratively carried on until the process objectives are met. *Process integration is regarded by (El-Halwagi, 1997, 2006) as a holistic and systematic way that consider the unity of the process for new (grass-root) or retrofit design.*

Environmental sustainability regulations, the rising cost of energy, raw material and waste treatment, and increasingly stringent emission regulations are among the factors that encourage the process industries to use process integration as a promising tool in resource conservation and sustainable process design (El-Halwagi, 2011; Foo, 2012; Foo et al., 2012; Klemes, 2013; Klemes et al., 2010). Two main areas of application are heat integration and mass integration. Following an early study of Hohmann (1986), Linnhoff and Flower (1978) proposed the concept of pinch analysis (pinch technology). Pinch analysis is now considered as a cornerstone for process integration and has been utilized in the synthesis of various processes such as that for heat exchanger (Kemp, 2007), mass exchanger (El-Halwagi and Manousiouthakis, 1989), hydrogen (Alves and Towler, 2002), water (Mann and Liu, 1999; Wang and Smith, 1994b), cooling water (Kim and Smith, 2001; Panjeshahi et al., 2009), and hot oil (Ataei et al., 2014). It also has been applied to carbon capture and storage (Tan et al., 2009), and carbon-constraint energy planning (Foo et al., 2008). The dedicated book for heat integration, first published by Linnhoff (1982) and recently revised by Kemp (2007), is a valuable user guide for the most common heat integration problems including heat exchange network synthesis, heat recovery targeting and selection of multiple utilities. The similarity between heat transfer and mass transfer leads to the development of mass exchanger network synthesis (El-Halwagi and Manousiouthakis, 1989), which later evolved into mass integration (El-Halwagi, 1997, 2006). Within the framework of mass integration, water network synthesis can be considered as a special case.

Water network can be designed through two approaches known as (1) optimization-based; or (2) insight-based. Problem dimensionality and computational effectiveness are the advantages of mathematical optimization especially when dealing with complex water distribution system including multiple contaminant, problem uncertainty, and compulsory and forbidden matches. However, in some cases the global optimality of the solution cannot be guaranteed because of the non-linearity of the problem. More importantly, since the engineering insight over the solution is not provided, it is less popular among industrial practitioners. Applying optimization technique to water network synthesis can be found in several literature (Bagajewicz, 2000; Gouws et al., 2010; Jeżowski, 2010).

2.2 Pinch analysis for water network synthesis

WPA offers a conceptual view upon the total system and gives engineers the full control to design the water network. The main power of this technique is in its ability to locate minimum utility targets (fresh water consumption and wastewater generation) with some basic data (contaminant concentration and flow rate) prior to detailed network design. This provides a base line for any water network to be synthesized. Certain water pinch technique were presented in the dedicated monograph by Mann and Liu (1999) and reviewed in the article by Foo (2009). The successful applications of pinch analysis for water network synthesis have been documented in various process industries such as pulp and paper (Tan et al., 2007; Tripathi, 1996), petrochemical (Mann and Liu, 1999), food processing

(Brouckaert and Buckley, 2000) municipal (Manan et al., 2006), and mineral (Deng and Feng, 2009).

2.2.1 Water network architecture

The water network in process industries mainly consists of three parts: pre-treatment processes, water using processes, and effluent treatment processes. In initial studies Takama et al. (1980) water network synthesis was looking at both effluent and water using processes as one unified system (so called total water network problem). The segregation of total water network to two subsystems (water using and effluent treatment processes) was proposed by Wang and Smith (1994b) who also developed WPA. This simplified the problem formulation outstandingly and the interaction between these two subsystems is further investigated in the later works (Kuo and Smith, 1998b). The inclusion of pre-treatment system to the total water network (called complete water network) was firstly reported by Ng et al. (2009).

The typical water network for most of industrial processes is depicted in Figure 2.1.

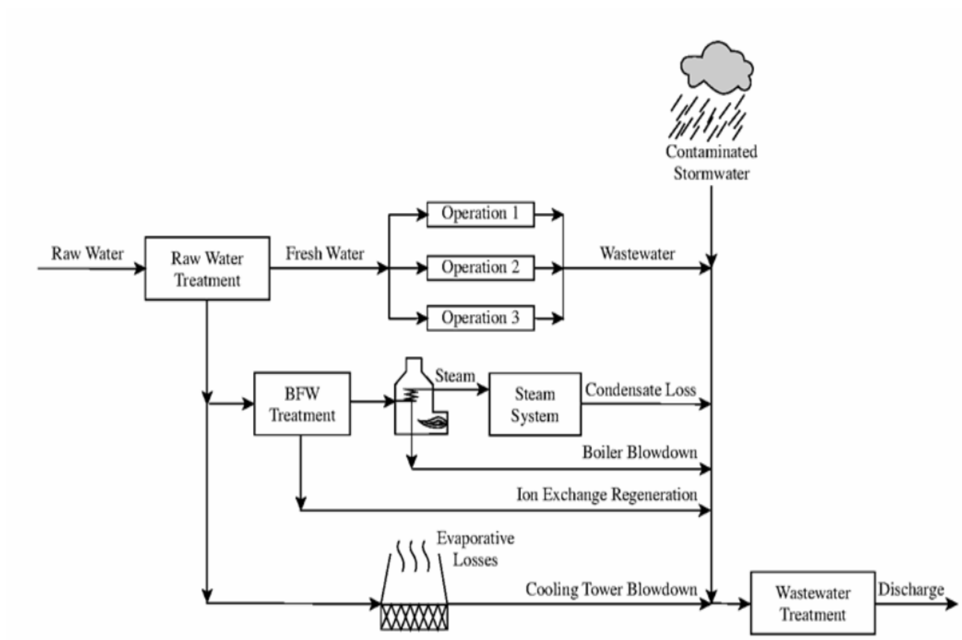

Figure 2.1.Typical water network system in process industries (Smith, 2005)

Water using processes can be further categorised as (a) processes uses (Operation 1, 2, 3) and (b) utility uses (cooling tower, boiler) (Mann and Liu, 1999; Smith, 2005). As shown, raw water is treated in preliminary water treatment facilities, then, it is fed to process uses and utility uses. Common sources of wastewater which include the effluent of process uses, condensate losses, boiler and cooling-tower blowdown is collected and directed to wastewater treatment system.

In this conventional water network, fresh water is directly utilised in all operations. However, it can be argued that not all of these units require fresh water because some of them may tolerate certain levels of contaminant concentration. Better water utilisation schemes should be designed to allow reuse/recycle between processes. Moreover, to design wastewater treatment process, there is possibly not necessary to collect all wastewater streams in centralised waste treatment facilities. More cost-effective wastewater treatment network is discussed later in this chapter.

2.2.2 Water minimization schemes

Minimizing water supply in water using processes can be achieved through water reuse, recycle and regeneration (Figure 2.2).

Reuse means that effluent from one water-using operation is passed to another operation without re-entering the operation from which it was generated (Figure 2.2a). Water reuse provides two-fold benefit: reducing both freshwater demand and wastewater generation of the system, simultaneously. However, this configuration is applicable only if Process II can accept the level of impurity from the outlet of Process I. Not all operations require high quality freshwater feed. One of the examples is multistage washing operation which high quality water should only be used only for final stages and it is possible to use low quality water in initial stages (Smith, 2005).

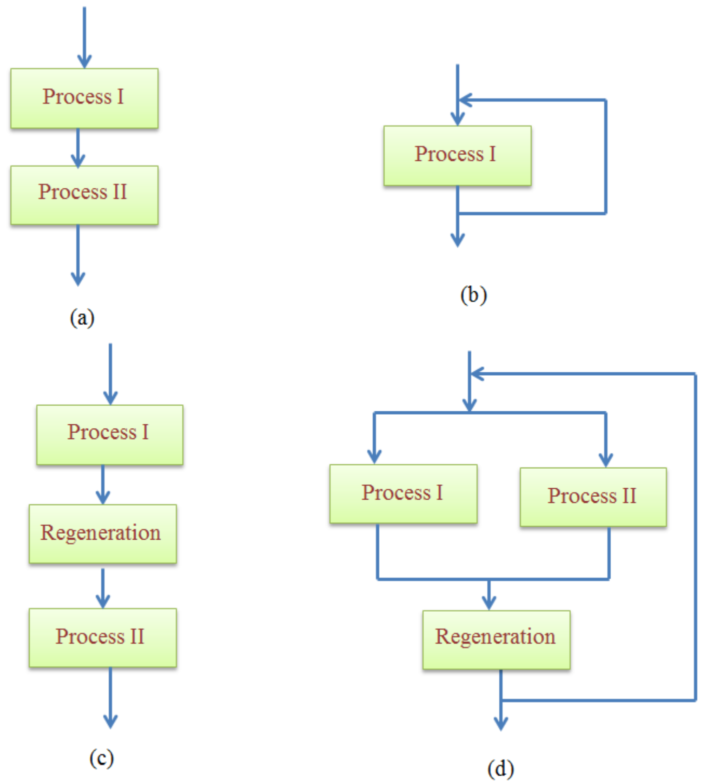

Figure 2.2.Various water minimization schemes (a) reuse (b) recycle (c) regeneration-reuse (d) regeneration-recycle

Recycle means that the effluent re-enter to the same process from which it is produced (Figure 2.2b). This scheme makes water going through the same operation several times. Although, more water saving is possible in compare with reuse configuration, the undesirable contaminant concentration will be built up and bring in problems for water network. For example the high amount of microorganism presenting in the network increases the risk of corrosion (Smith, 2005).

Regeneration scheme allows the effluent to be partially treated before either reuse (Figure 2.2c) or recycling (Figure 2.2d) takes place (Wang and Smith, 1994b). In contrast to pure reuse/recycle, more space for freshwater saving is achievable within regeneration-reuse/recycle configuration. However, a capital investment is required for the regeneration unit to be installed in the network. Therefore, economical evaluation in water regeneration network is an important issue to be considered. Regeneration-recycle gives an opportunity to save water resources to the maximum extent, that is, in some cases it is possible to achieve zero liquid discharge (Deng et al., 2008) under this scenario, hypothetically. However, since recycling imposes the problem to the network, the technical feasibility of this configuration should be assessed before implementation.

2.2.3 Wastewater treatment network

In the past, most design studies dealt with centralized effluent treatment networks (Figure 2.3a) rather than distributed wastewater treatment systems (Figure 2.3b). In a centralized system, all effluent streams from various operations are collected and undergo central treatment process. In contrast, in distributed effluent systems, streams from different processes are segregated and treated separately.

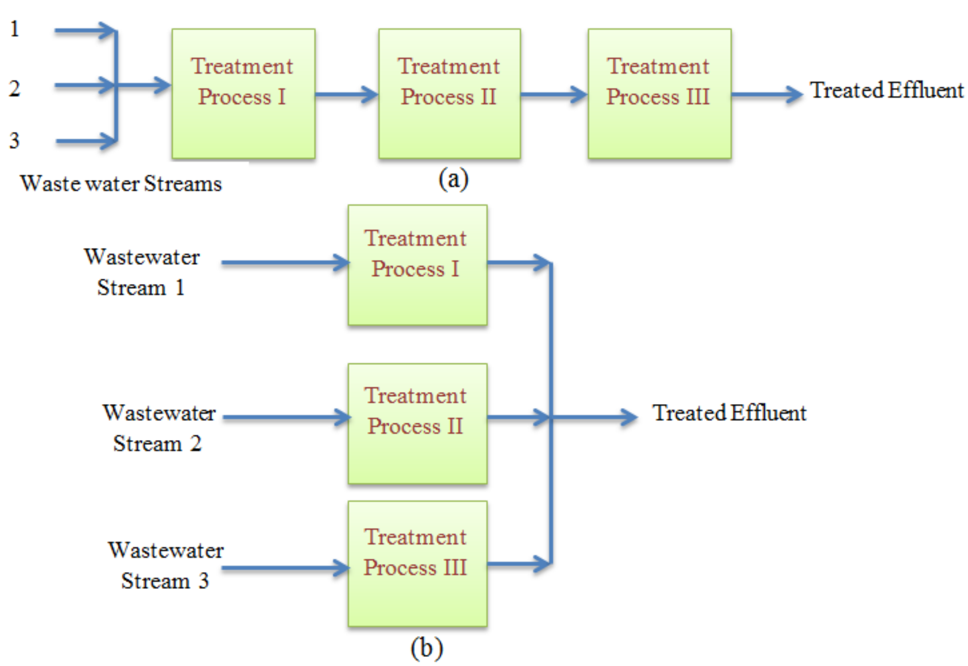

Figure 2.3.Various water treatment systems (a) centralized system (b) distributed network

The capital cost and operating cost of the treatment process is closely related to two factors: the inlet wastewater flow rate and its contaminant concentration. The treatment process in distributed system takes lower inlet flow rate with higher inlet contaminant concentration of wastewater. For a given mass load of contaminant to be treated, this kind of system is more economical and cost-effective By applying WPA, the optimal distributed water treatment system can be achieved (Mann and Liu, 1999; Wang and Smith, 1994a).

2.2.4 Statement of problems - Fixed Load vs Fixed Flow rate

Water network model is classified into two main categories named mass-transfer (also called quality controlled, fixed load) problem and non-mass-transfer units (also called sinks and sources, quantity controlled or fixed flow rate operations) problem (Bagajewicz, 2000). The terminologies of Fixed Load (FL) and Fixed Flow rate (FF) are chosen in this thesis to represent these two kinds of problems.

Fixed Load is modelled as mass transfer units. In this model, inlet and outlet water flow rate to the particular process are redeemed as the same. Typical examples of such processes include: vessel cleaning, solvent extraction, gas absorption, etc. On the other hand, Fixed Flow rate problems involve operations where mass transfer does not necessarily take place. This kind of operation includes boilers, cooling tower, filters etc. Water flow rate entering the process is not essentially equal to outlet flow rate as water loss/gain may occur. Models in this category may deal with both FL and FF problems in the targeting stage.

- ***Fixed load problems***

The main focus in FL problem is the impurity load removal from contaminated streams where water is mainly used as mass separating agent (Figure 2.4).

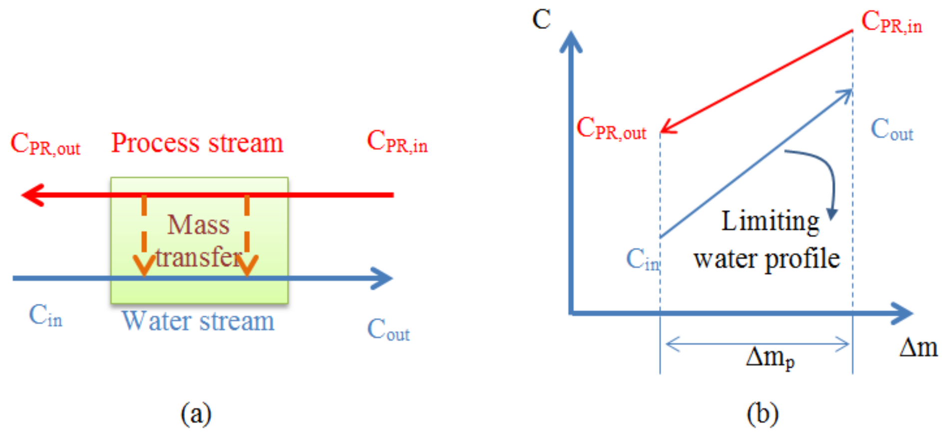

Figure 2.4.Fixed load problem presentation (a) water using process where water is used as mass separating agent (b) limiting water profile

The problem statement is given as follows (Smith, 2005; Wang and Smith, 1994b):

- There is a number of water using processes called PROCESS or P = (1, 2,.., Np). Each process has a rich stream with an impure inlet concentration of $C_{\mathrm{PR,in}}$ and outlet concentration of $C_{\mathrm{PR,out}}$. The process requires an impurity removal load of Δm_p (Figure 2.4a).
- Water may enter and leave the process at maximum inlet (C_{in}) and outlet (C_{out}) concentrations respectively dictated by process impurity concentration (limiting water profile) (Figure 2.4b). Considering the single impurity (contaminant concentration), this concept provides the opportunity to reuse water among the processes.
- External fresh water source(s) should be introduced to satisfy the impurity removal requirement of the process. The required water for every process is calculated by Eq. 2.1:

$$F_p = \frac{\Delta m_p}{C_{out} - C_{in}} \qquad (2.1)$$

➢ ***Fixed flow rate problems***

In the fixed flow rate (FF) problem, the inlet and outlet flow rate for the process may not be uniform. Hence, the main constraint in such problems is the flow rate not the impurity load removal. Synthesis tools developed in FF model address the problem from the water sink and source perspective (Figure 2.5).

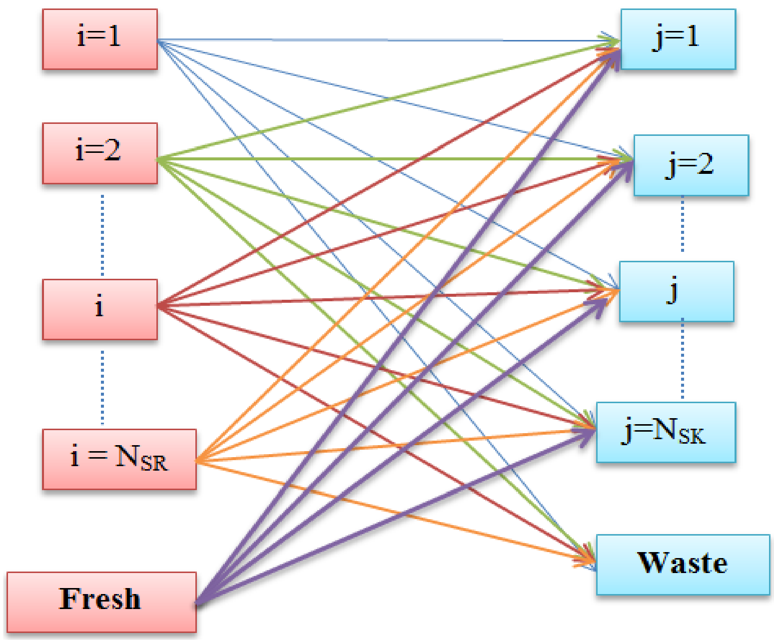

Figure 2.5.Source/sink representation of water network

The general definition is as follows (El-Halwagi, 1997, 2006; Foo, 2012):

- Processes needing water are designated as SINKS or SK_j (j=1, 2, …, N_{SK}). Each SINK has a given flow rate, F_j and inlet concentration of targeted impurity, C_j, which must satisfy: $C_j^{min} \leq C_j \leq C_j^{max}$, where C_j^{min} and C_j^{max} are the lowest and highest concentration limits of the targeted impurity.
- Water-generating processes reused or recycled to SINKS are designated as SOURCES, or SR_i (i= 1, 2,…, N_{SR}), with a given flow rate of F_i, and impurity concentration of C_i.

- External freshwater feed(s) should be introduced to fulfil the requirement of sinks flow rate with specific concentration. Unused water from process sources will be directed to the waste.

➢ ***Conversion of limiting water data between FL and FF models***

In water network synthesis, the overall objective is to minimize external freshwater requirement and waste generation. There is a possibility to convert FL model to FF and vice versa (Figure 2.6).

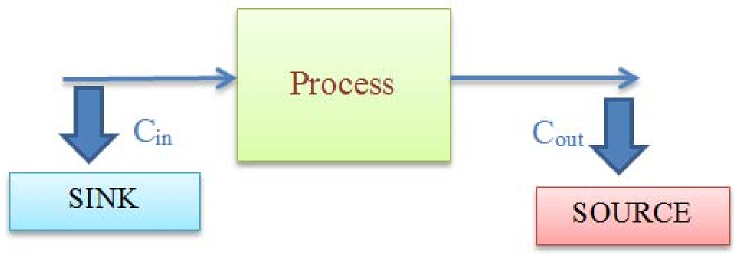

Figure 2.6.Conversion of fixed load model to fixed flow rate model

When converting FL to FF, the inlet and outlet in FL operation can be considered as process sink and source of FF model. Because a process does not necessarily have one single inlet and outlet stream, the sink/source representation can easily take flow rate loss/gain into account. Most of the water pinch targeting methodologies using FF model are capable of handling water network synthesis in a broader sense. These techniques, hence, are more versatile than those developed for FL problems. However, one should note that the conversion between FL and FF model only is applicable for single contaminant cases.

2.3 Targeting techniques

The power of Pinch Analysis is in its ability to locate a minimum utility targets prior to detailed network design. Similar to other pinch analysis techniques (e.g. heat and mass pinch analysis), WPA has two main stages: freshwater and wastewater flow rate targeting (Analysis) and network design (Synthesis).

Targeting aims to identify the minimum utility requirement and key parameters in water utilization scheme and effluent treatment network with given basic information on impurity concentration and water flow rate limitations. Key parameters in reuse/recycle scheme are freshwater flow rate, wastewater flow rate, and reuse/recycle pinch concentration. In regeneration scheme, in addition to pre-mentioned variables, inlet regeneration and post (outlet) regeneration concentrations along with regenerated water flow rate and regeneration pinch concentration are essential to be set. For distributed effluent network, the minimum treatment flow rate and its associated pinch point can be targeted.

Targeting methodologies are classified, compared, and evaluated for reuse/recycle and regeneration-reuse/recycle water network in the following sections. The existing research gaps and the contribution of this study to fill the gaps are described.

2.3.1 Reuse/recycle water network

Figure 2.7 portrays the development of water pinch targeting methodologies in reuse/recycle water network. Three different categories are considered to classify the methods namely, graphical, numerical, combined graphical and numerical.

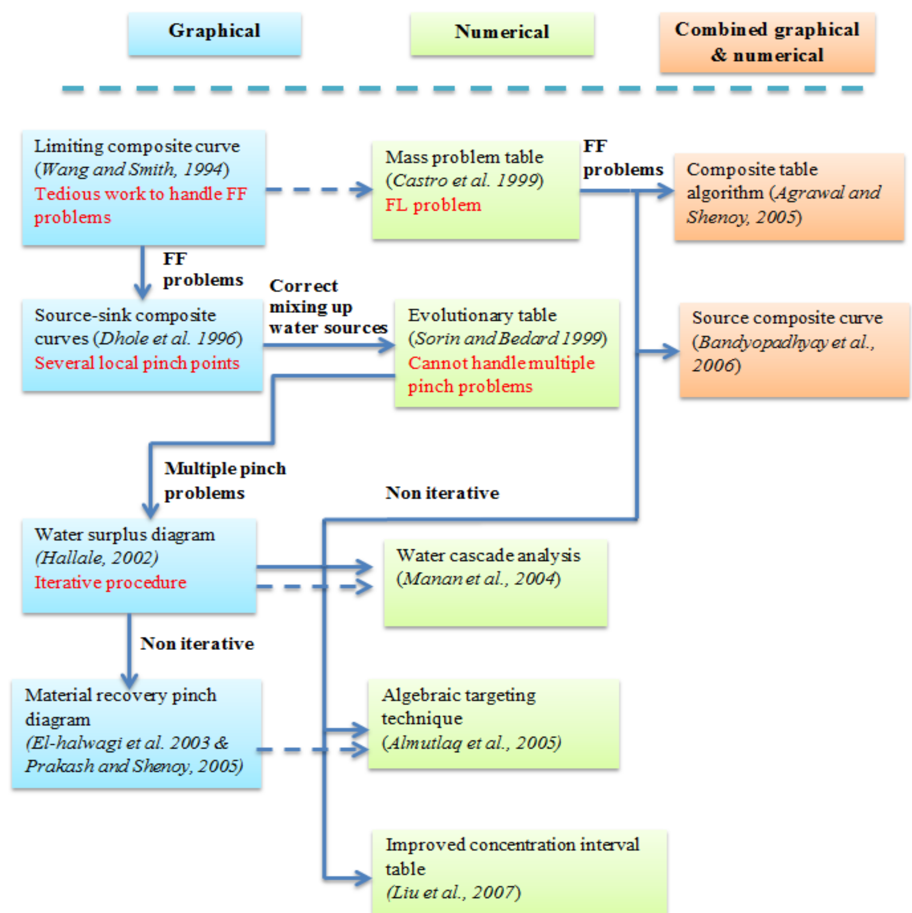

Figure 2.7.Development of pinch targeting methods for reuse/recycle water network

The limitation of each method (if any) is shown in red. Approach(s) proposed to address these limitations are connected with solid arrows. Dashed line links two methods with similarities.

The seminal work of water network synthesis applying pinch analysis was contributed by Wang and Smith (1994b). This graphical targeting method is well known as limiting composite curve (LCC). To construct the LCC, all processes are plotted on a mass load (x-axis) and contaminant concentration (y-axis) diagram. Within each concentration interval, the mass load of all operations is accumulated. Mass Problem Table (MPT) (Castro et al., 1999; Mann and Liu, 1999) is a numerical targeting method similar to the LCC (Wang and Smith, 1994b). Although both graphical and numerical targeting methods lead to the same result, they are complementary. Graphical targeting methods provide insight to the problem while numerical analyses are more useful in terms of computational effectiveness. The basic concept underlying these seminal works is that, all water-using processes are modelled as FL operations. The water flow rate through the process was assumed to be constant so, the water loss/gain was neglected. Water loss/gain is a common practice in the real process industries. Although, Wang and Smith (1995) water loss/gain in their later work, the proposed procedure is very tedious to handle, where, water supply composite curve needs to be adjusted iteratively to cater for water loss/gain. Therefore, several FF targeting methods were developed later.

By developing Source-Sink Composite Curves method for both FL and FF operations, Dhole et al. (1996) addressed this limitation in first principal. Later it was found that this approach results in several local pinch points and does not necessarily guarantee the correct minimum targets. It appears that Source-Sink Composite Curves method cannot systematically address the mixing up of water sources. To overcome this limitation, Evolutionary Table was developed by Sorin and Bédard (1999). However, this method is unable to handle multiple pinch problems.

Water Surplus Diagram (WSD) (Hallale, 2002) was the first promising tool for targeting global water operations. Hallale (2002) used this method for both FL and FF operations and multiple pinch problems. This method consists of two subsequent stages: the plot of source and sink composite curves and the construction of water surplus diagram. These two steps need to be repeatedly conducted until the constructed WSD completely lies on the positive (right) side of the diagram and touches the concentration axis at pinch point(s). Hence, the shortage of this technique is its iterative characteristic in order to set the targets. However, this method made contributions to other pinch analysis techniques for targeting the FF problems by revealing two key facts:

- Pinch point(s) is always created on one or more of the source concentrations;
- The necessity of two graphical plots dictates that two constraints should be considered, i.e. the flow rate or quantity (for source-sink

composite curves) and the impurity removal (for water surplus diagram).

To deal with the iterative characteristic of WSD, a graphical targeting method, the Material Recovery Pinch Diagram (MRPD), was firstly proposed by two different groups of researchers (Prakash and Shenoy, 2005b) (El-Halwagi et al., 2003). Later, several numerical methods were also developed such as: Water Cascade Analysis (WCA) (Manan et al., 2004), Algebraic Targeting Method (Almutlaq and El-Halwagi, 2007), and Improved Concentration Interval Table (Liu et al., 2007) . Although these targeting methods are all algebraic, the basic concept behind these techniques is completely different. WCA was developed based on the concept of WSD (Hallale, 2002). Almutlaq and El-Halwagi (2007) developed the Algebraic Targeting Method using the idea of MRPD and the Improved Concentration Interval Table is the extension of MPT (Castro et al., 1999) to be capable of addressing FF problems.

Furthermore, two hybrid, non-iterative methods also put forward known as Source Composite Curve (Bandyopadhyay et al., 2006) and Composite Table Algorithm (CTA) (Agrawal and Shenoy, 2006). Source Composite Curve was proposed to analyse the interaction between water-using processes and waste treatment facilities (total water network problem). Therefore, it is the only method which targets the wastewater flow rate ahead of freshwater and can set the wastewater contaminant concentration without the need of further calculations. CTA developed by Agrawal and Shenoy (2006) is more analogous to the early work of pinch analysis (i.e. limiting composite curve). Hence, like LCC can be used for various water network synthesis problems, CTA has the potential to be further extended as a comprehensive targeting method for FL, combined FL and FF, and multiple pinch problems. This has been accomplished in this study.

Under reuse/recycle water network synthesis, two specific problems are brought into our particular attention: the multiple utility system and the threshold problem.

(a) Multiple utilities systems

Most of the aforementioned targeting methods initially were proposed with the assumption of pure freshwater supply. However, in reality, multiple utilities with various contaminant concentrations may be available for service. These outsourced feedwater can consist of borehole water, river water, or imported water etc. Wang and Smith (1995) started with FL problems to set the target for multiple utilities by employing the LCC method . Later, the WCA (Foo, 2007), and the MRPD (Alwi and Manan, 2007), were extended to target the flow rates for multiple freshwater sources with different contaminant concentrations in a broader sense (considering both FL and FF problems). However, none of these studies can guarantee the economic optimality. The lower quality freshwater source(s) is assumed to be virtually free of charge. A prioritized cost factor was suggested by Shenoy and Bandyopadhyay (2007) to find the optimum economic scenario of water utilities. Considering the prioritized cost, the Improved Problem Table, an extended version of CTA was developed by Deng and Feng (2011) to study multiple utility problems.

(b) Threshold problems

Threshold problem in water network synthesis is very rare but realistic. Cases can be (a) water network requiring freshwater feed without generating waste disposal or; (b) wastewater produced in the network with no freshwater feed. In very special scenario, (c) neither freshwater is needed nor wastewater discharges. These kinds of problems in the FF model initially were addressed by Water WCA and MRPD (Foo, 2008). Later, Alwi and Manan (2007) extended MRPD approach to target the flow rates of utilities for the “threshold problem without water discharge”.

It is worth mentioning that regeneration scenarios for water saving are not feasible in the threshold problems due to insufficient amount of process sources (Alwai and Manan, 2007). Therefore, the determination of these problems is essential before designing regeneration-reuse/recycle water network. The following section describes the development of pinch targeting method in regeneration-reuse/recycle water network.

2.3.2 Regeneration-reuse/recycle water network

Water regeneration means that the wastewater is partially or totally purified using any treatment techniques. The regenerated water then can be either reused to the other processes or recycled back within the network. In compared to pure reuse/recycle scheme, regeneration leads to less freshwater consumption and wastewater generation. The regeneration units falls into two broad categorizes namely, fixed post (outlet) regeneration concentration or specified removal ratio type (Wang and Smith, 1994b). Removal ratio of purification facility is defined as the impurity load picked up by treatment process to the total inlet impurity load.

The early contribution on regeneration targeting was made by Smith and his colleagues (Kuo and Smith, 1998a; Wang and Smith, 1994a, b) . Wang and Smith (1994b) extended LCC method to be applicable for regeneration targeting. The freshwater is consumed in some processes until it reaches the reuse/recycle pinch concentration. Then, it is treated in the regenerator to meet the outlet regeneration concentration before being reused or recycled further. In regeneration-reuse scheme, the freshwater and regenerated water flow rates are identical. On the other hand, for the regeneration-recycle network, freshwater flow rate is lower than the regeneration flow rate due to recycling permission. Later, it was observed that considering reuse/recycle pinch concentration as a regeneration concentration is not generic enough to set the targets (Kuo and Smith, 1998a; Mann and Liu, 1999). Pinch concentration may be relocated to another LCC's turning point after the regeneration takes place. In other words, the minimum freshwater target cannot be found under the pre-specified assumption.

To address this limitation, Kuo and Smith (1998a) proposed the decomposition of a process into regeneration and freshwater regions. LCCs are constructed in both regions and minimum flow rate targets (freshwater and regenerated water) are located. However, this approach needs an iterative procedure to migrate the processes between each region. It causes the complexity to the analysis. Mann and Liu (1999) suggested the existence of multiple pinch points to target the key parameters in regeneration-recuse/recycle problems. The regeneration concentration may be either below or above reuse/recycle pinch concentration according to the shape of LCC. This concept was adopted by other researchers and further studies have been conducted in the development of sequential optimization method and the extension of mass problem table (Deng and Feng, 2011; Feng et al., 2007). All of the aforementioned techniques are restricted to the FL model, therefore, cannot handle water loss/gain within the network.

The first guideline for regeneration placement in FF problems, which can account for flow rate loss/gain, was proposed by Hallale (2002). In his work, the network was divided into below pinch (surplus of water) and above pinch (deficit of water) regions via WSD method. It was suggested that, in order to reduce the overall freshwater demand, it is better to place the regeneration unit across the pinch concentration. In this way, wastewater will be collected from surplus region, purified and fed to the region with the deficit of water. Therefore, it is possible to achieve the biggest saving in both freshwater requirement and wastewater generation. Following this guideline MRPD and WCA have been used to locate the regeneration unit (El-Halwagi, 2006; Foo et al., 2006; Manan et al., 2004).

Nonetheless, all of these methods cannot locate the minimum freshwater, wastewater, and regenerated flow rates simultaneously. This limitation was rectified by Ng et al. (Ng et al., 2007b, 2008) through the proposed ultimate flow rate targeting method. Because this method was developed on the basis of Kuo and Smith's (1998a) flow rate allocation , it also needs iterative procedure and is tedious to handle.

Most of the above-mentioned studies are on the assumption of fixed post-regeneration concentration. Very recently, Xu et al. (2013) made an effort to relax this assumption and to predict the relationship between regeneration pinch and post-regeneration concentration. However, the work did not consider the whole range of feasible post-regeneration concentration and only FL operations was addressed. Knowing the fact that the post-regeneration concentration has a dominant influence to the total cost of network, it is essential to analyse the effect this parameter in further details.

A water network with zero liquid discharge can be the specific case of the regeneration-recycle water network (Bandyopadhyay and Cormos, 2008; Deng et al., 2008). If all processes in the water network are FL operations (without flow rate loss/gain), meeting zero freshwater requirement also means achieving zero water disposal. Placing the regenerator with post-regeneration concentration lower than inlet concentration of all processes, it is possible to obtain closed circuit configuration. Wastewater is treated to some extent in the regeneration unit and then recycles back through the network. For the network with total water loss, zero wastewater discharge is still achievable if the amount of loss is compensated by freshwater feed. Deng et al. (2008) employed CTA as a targeting tool to analyse such a problem. Although, attaining a zero discharge network is very interesting in terms of environmental sustainability, it is practically very difficult and expensive due to, for an example, the accumulation of undesirable contaminates.

The performance of water regeneration unit is judged by two criteria (1) specified post-regeneration concentration; (2) specified removal ratio (RR). Most of pinch analysis methods considered the first criterion for targeting regeneration-reuse/recycle network (Agrawal and Shenoy, 2006; Bai et al., 2007; El-Halwagi, 2006; Foo et al., 2006; Hallale, 2002; Kuo and Smith, 1998a; Manan et al., 2004; Mann and Liu, 1999; Ng et al., 2007b, 2008). A little attention has been paid to the RR type regenerator (Bandyopadhyay and Cormos, 2008; Wang and Smith, 1994b). The work of Wang and Smith (1994b) dealt with very simple single pinch problem and it is restricted to fixed load water operations. Although, source composite curve (Bandyopadhyay and Cormos, 2008) can handle RR type regenerator, it only locates the target for regeneration-recycle network and very special case of zero liquid discharge.

2.4 Network design

All water-using processes are connected together to form the process flow sheet through the network design. Note that, all targets should be satisfied through this subsequent stage. The heuristic proposed for the network design may be different based on the characteristics of targeting.

Network design is a degenerated problem. There exist several alternative designs for pre-determined targets. Varity of water network design have been developed since the establishment of pinch analysis theory in 1994. These are broadly classified to FL and FF problems and mapped on the basis of their contributions to the water network problems in Table 2.1. It can be seen that not all the methods find applications to specific problems. For instance, Olesen and Polley (1997) used the load table method to design the reuse/recycle water network without considering regeneration and waste treatment problems. This table somehow indicate possible research gaps. Some of the network design methodologies are dependent on the targeting stage, while others are not (those shown in bold). Water Grid Diagram, Water Main Method, and Mass Content Diagram are related to LCC targeting (Wang and Smith, 1994b) method. Three Design Rules, Nearest Neighbor Algorithm, and Network Allocation Diagram are proposed based on the concept of MRPD method (El-Halwagi et al., 2003; Prakash and Shenoy, 2005b). The Concentration Interval Analysis is the design tool for Improved Concentration Interval Table method (Liu et al., 2007).

For the design method independent from targeting, the two stages of pinch analysis can be achieved simultaneously. However, the application of these methods is not as simple as those which are dependent on the targeting stage. In fact, since the conceptual insight provided from the targeting stage is very valuable for network design and process changes, targeting has become a preferred practice in most pinch analysis studies. The network design tools thereafter highly correspond to the targeting stage.

Table 2.1.Comparison of water network design methods (Foo, 2009)

Design methods \ Problems	Reuse/ recycle	Water regeneration	Wastewater treatment /Total water network
FL problem			
Water Grid Diagram	(Mann and Liu, 1999; Wang and Smith, 1994b)	(Mann and Liu, 1999; Wang and Smith, 1994b)	(Kuo and Smith, 1997; Mann and Liu, 1999; Wang and Smith, 1994a)
Load Table	(Olesen and Polley, 1997)		
Water Main Method	(Kuo and Smith, 1998b; Smith, 2005)	(Cao et al., 2004; Kuo and Smith, 1998b; Smith, 2005)	(Mann and Liu, 1999)
Mass Content Diagram	(Mann and Liu, 1999)	(Mann and Liu, 1999)	(Mann and Liu, 1999)
Concentration Interval Analysis	(Liu et al., 2007)		
Water Source Diagram	(Gomes et al., 2007)	(Gomes et al., 2007)	
Three Design Rule	(Prakash and Shenoy, 2005b)		
FF problem			
Source Sink Mapping Diagram	(El-Halwagi, 1997, 2006)	(El-Halwagi, 1997, 2006)	(El-Halwagi, 1997, 2006)
Source Demand Approach	(Polley and Polley, 2000)		
Load Problem Table	(Aly et al., 2005)		
Nearest Neighbor Algorithm	(Prakash and Shenoy, 2005b)	(Agrawal and Shenoy, 2006)	(Ng et al., 2007a)
Network Allocation Diagram	(Alwi and Manan, 2008)		

In contrast with targeting stage, the design methodologies developed for FF problems cannot handle FL problems effectively. Although the network may meet the minimum freshwater flow rate target, it is relatively complicated, and the freshwater flow rate going through every process is quite high (Prakash and Shenoy, 2005b). Recently, Shenoy (2012) developed a method, the enhanced nearest neighbor algorithm, to deal with both FL and FF problems. It was applied for reuse/recycle water network as well as for zero liquid discharge network with inclusion of regeneration unit.

Three Design Rules of Prakash and Shenoy (2005b) was developed for reuse/recycle water network design in FL problems. Moreover, it was utilised to achieve zero liquid discharge for regeneration-recycle water network (Deng and Feng, 2011; Deng et al., 2008). However, the capability of this method to address total regeneration-reuse water network in FL model has not been fully demonstrated.

Finally, after the preliminary network was formed, a simplified network can be obtained using network evolution techniques (Ng and Foo, 2006; Prakash and Shenoy, 2005a; Wang and Smith, 1994b) .

2.5 Summary

In this chapter, the milestone literature contributed to water network synthesis problem applying pinch analysis, has been classified and reviewed (to the best of the writer's knowledge). Although methodologies have been developed for various problems, some issues have not been addressed, explored or investigated

- A robust targeting method, which can handle diverse problem in reuse/recycle scheme both algebraically and graphically, was not explored.
- In regeneration problems, non-iterative, hybrid graphical and numerical targeting method which is capable of addressing global water operation has not been developed. Moreover, most of targeting methodologies are restricted to fixed post-regeneration criteria and no economic evaluation is studied.
- The best option for pure freshwater minimization in the "threshold problem without waste discharge" is the harvesting impure utilities. However, there is no systematic analysis in the literature.

In this work, we conduct studies to bridge these literature gaps. The background methodologies which will be used to address the aforementioned limitations will be described in detail in Chapter 3.

3. BACKGROUND METHODOLOGIES

In this chapter, the detailed procedure of several water pinch targeting methods, Limiting Composite Curve (LCC), Material Recovery Pinch Diagram (MRPD), Water Cascade Analysis (WCA), and Composite Table Algorithm (CTA), are described to accommodate the necessary knowledge for the understanding of further methodology development presented in this research.

WPA study was started in 1994 with Limiting Composite Curve as targeting method. However, applying LCC for realistic cases with flow rate loss/gain appeared to be a cumbersome activity. To deal with this drawback, several targeting methods based on source/sink perspective were developed. Among them, Composite Table Algorithm is a hybrid approach. Both physical insight and numerical accuracy can be achieved. Additionally, the graphical presentation of CTA is similar to LCC method and LCC, as a well-established method, has its power in targeting stage. Therefore, there is a potential to extend CTA for various water network problems. The improvement of CTA to be a comprehensive water pinch targeting technique is aimed for this study.

The introduction of impure utilities to save pure freshwater source for the threshold problem without waste discharge is another objective of this study. The threshold problems are easily recognisable via MRPD. Thus, MRPD is employed for proposing different scenarios in order to introduce impure utilities. Furthermore, WCA is also utilised as a complementary tool of MRPD to provide numerical accuracy.

For design stage, two well-known water network design techniques named as Nearest Neighbor Algorithm (NNA) and Three Design Rules (TRD) will be introduced. While the former is applicable for fixed flow rate problems, the latter can handle fixed load problems. However, the basic information underlying these methods is the same. Since diverse problems are investigated in this study, based on the characteristic of the problem, either of these methods will be used for network design.

To introduce each of these techniques explicitly, limiting data from literature examples are adopted. Results obtained via these methods are compared and elaborated. This chapter aims to provide sufficient information for the reader to understand the rest of thesis.

3.1 Targeting

As mentioned in the preceding chapters, the first stage for most pinch analysis practices is targeting. Within this stage, prior to the detailed water network design, the key parameters are identified based on the primary data (operation's contaminant concentrations and flow rates). In the following, four targeting methodologies: LCC, MRPD, WCA, and CTA will be explained in detail.

3.1.1 Limiting Composite Curve

The Limiting Composite Curve (LCC) method is the seminal work in the area of WPA for targeting minimum freshwater and wastewater flow rates (Wang and Smith, 1994b). To construct the LCC, the limiting data for individual processes are plotted on the impurity concentration vs. mass load diagram. The impurity loads are then summed up in every concentration interval to present the water network as the overall system.

Consider Example 3.1 with the limiting data given in Table 3.1. These data are collected by considering the maximum reuse opportunity within the network. Hence, both inlet (C_{in}) and outlet (C_{out}) contaminant concentrations for every process are set to the maximum allowable values, that is, the mass transfer can still occur. With the given water flow rate (F_p) of each process, the impurity removal (Δm_p) can be calculated using Eq 2.1.

Table 3.1.Limiting data for Example 3.1(Wang and Smith, 1994b)

Process, P_p	Δm_p (kg/h)	C_{in} (ppm)	C_{out} (ppm)	F_p (ton/h)
1	2	0	100	20
2	5	50	100	100
3	30	50	800	40
4	4	400	800	10

To form the LCC, the following procedure should be used (Mann and Liu, 1999; Smith, 2005; Wang and Smith, 1994b):

1) Plot each process in concentration (C) vs. mass load (Δm) diagram. While the y-axis is the absolute concentration, the x-axis corresponds to the relative mass load. Therefore, each process begins from where the prior process ends (Figure 3.1a).
2) Draw horizontal lines at the inlet and outlet concentrations of each process so that, the vertical axis (y-axis) is divided into several concentration intervals (Figure 3.1a).
3) Sum up the mass load of all processes in every concentration interval and draw a new line to present a system as a single entity results in the LCC formation (black line in Figure 3.1b).

Then, to target water reuse opportunity, water supply line (red line in Figure 3.1b) is introduced. The line is drawn from the origin, and it is rotated anti-clockwise until the pinch point is formed. Note that, for this example, pure freshwater is assumed. For this issue, the 0 ppm contaminant concentration is considered as a pivot point to plot water supply line. The inverse slope of fresh water supply line identifies the minimum freshwater flow rate requirement of the network. This network needs 90 ton/h of freshwater and the network's bottleneck encounters at the 100 ppm contaminant concentration. Since all processes are assumed to be fixed load operations (no flow rate loss/gain), the wastewater flow rate leaves the network is also 90 ton/h. One other valuable insight from the LCC method is the targeted contaminant concentration in wastewater, which is indicated by the end point of freshwater supply line (455.6 ppm for this example).

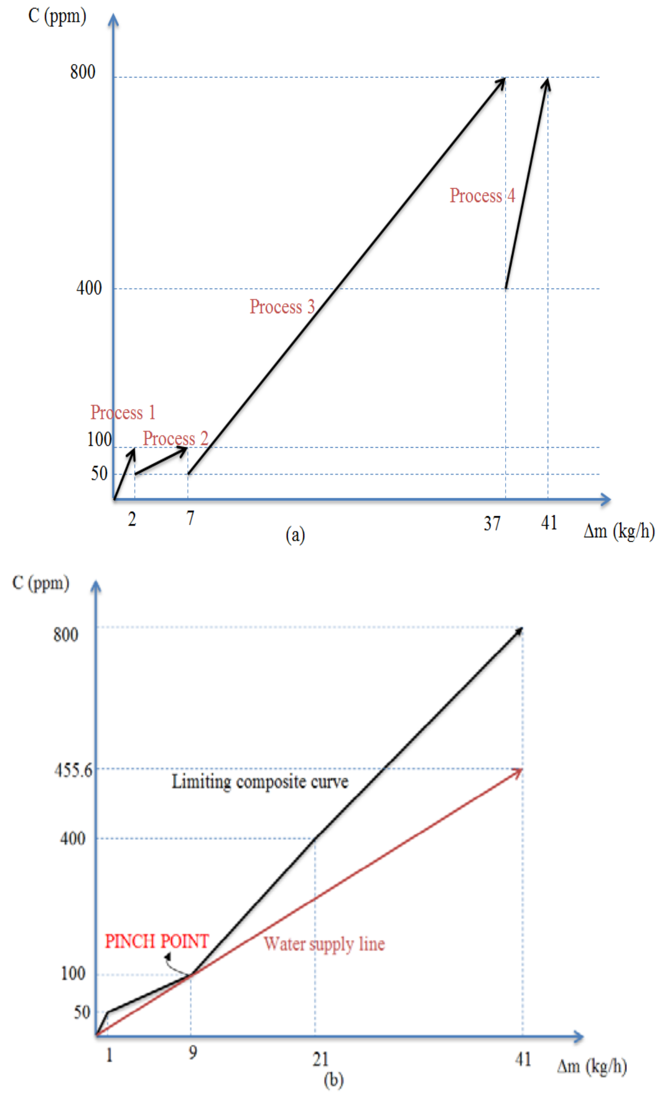

Figure 3.1.The procedure for construction of LCC (a) presentation of every process in impurity load vs. contaminant concentration diagram (b) set up the targets (Example 3.1)

For comparison, if reuse opportunities are not considered, pure freshwater will be needed for each individual process to remove specified impurity. The corresponding flow rate can be calculated using Eq 3.1 as below:

F1= 2000/ (100-0) = 20 (ton/h); F2=5000/ (100-0) = 50 (ton/h) and the same for F3=37.5 (ton/h), and F4=5 (ton/h)

Therefore, the total freshwater flow rate will be 112.5 (ton/h).

It is clear that, utilising the LCC method, through reuse/recycle configuration, it is possible to save pure freshwater consumption and wastewater generation up to 25% for this example.

The LCC method was used for targeting multiple utilities problem later (Wang and Smith, 1995) . The contaminant concentrations of impure utilities are given. Moreover, the LCC set the minimum allowable mass transfer constraint. Hence, the impure utilities concentration should be pinpointed on the LCC. Then, drawing the water supply line from origin to the points, which is corresponding to the impure utilities concentrations, identifies the minimum flow rates targets. The main assumption is that the better quality water source, the more expensive it is. Therefore, water utilities should be minimized from higher to lower qualities in order. However, this assumption, which may not find the economic optimum scenario, was relaxed later through the prioritise cost index (Shenoy and Bandyopadhyay, 2007).

The schematic diagram for targeting multiple utilities applying LCC is illustrated in Figure 3.2. Two freshwater sources, Demin and Portable water, are considered. *Cpot* associated with the contaminant concentration of portable water.

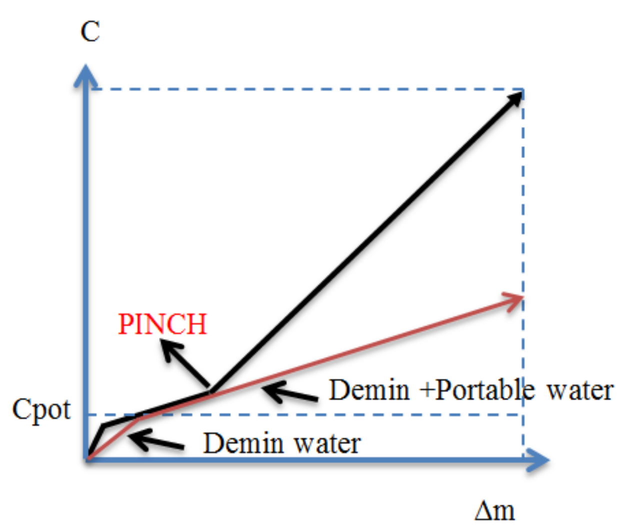

Figure 3.2.Multiple utilities targeting using LCC

The LCC method was also modified for targeting of regeneration-reuse/recycle water network (Wang and Smith, 1994b) . The targeting procedure is depicted in Figure 3.3. The way for LCC construction is the same as described earlier. However, the water supply line has to be changed, since it represents the demand for water before and after regeneration unit.

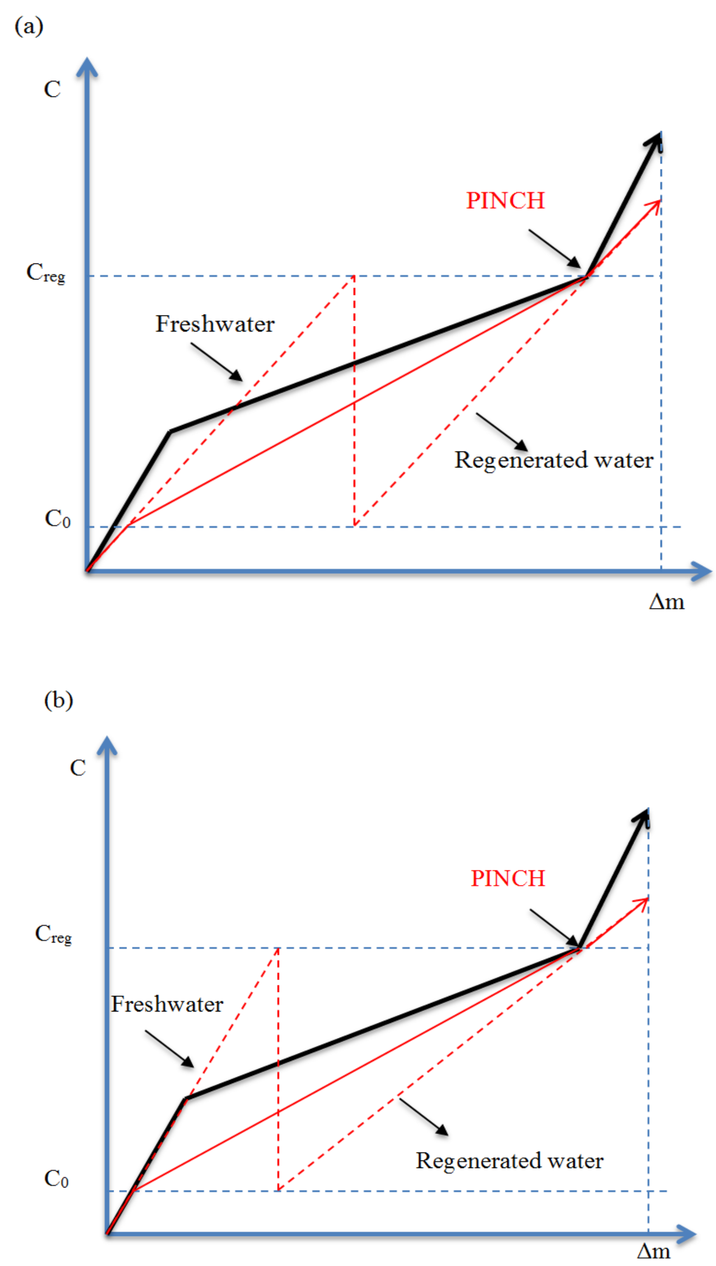

Figure 3.3.LCC method for targeting (a) regeneration-reuse water network (b) regeneration-recycle water network

As shown, the freshwater is used in some processes until it reaches the regeneration concentration (C_{reg}), then it is treated to the post-regeneration concentration (C_0) before being reused /recycled in other processes. For regeneration-reuse (Figure 3.3a), the freshwater and regenerated water segments should have the same slope. However, for regeneration-recycle (Figure 3.3b), the fresh water flow rate would be lower than regenerated water. Therefore, the slope of fresh water segment, which is higher than regenerated water segment, is restricted by the LCC.

For Example 3.1, assuming the C_0 to be 5 ppm, it is possible to reduce the freshwater demand to 46.2 ton/h or 20 ton/h, by applying regeneration-reuse or regeneration-recycling water network, respectively.

To utilise this method, the optimum regeneration concentration should be equal to the reuse/recycle pinch concentration (Cpinch = C_{reg}). However, as observed (Bai et al., 2007; Feng et al., 2007; Kuo and Smith, 1998a; Mann and Liu, 1999), this rule may not be held correct for some multiple pinch cases and the minimum freshwater flow rate would not be targeted.

Some extensions to LCC were proposed for flow rate loss/gain (Wang and Smith, 1995). Although limiting composite curve remains unchanged, the water supply line should be adjusted to reflect the water loss/gain. This procedure is an iterative task and very cumbersome. This was dealt with later by other targeting techniques for fixed flow rate problems. Some of these are described in the following.

3.1.2 Material Recovery Pinch Diagram

This is the first graphical targeting technique developed for fixed flow rate problems to cope with the iterative steps of water surplus diagram method (Hallale, 2002). It is interesting to note that, this method is individually developed by two different research groups, El-Halwagi et al. (2003) from US and Prakash and Shenoy (2005b) in India.

Example 3.2 from Polley and Polley (2000) is chosen to describe the detailed procedure of MRPD method. The limiting data is listed in Table 3.2. As mentioned in Chapter 2, targeting for fixed flow rate problems is addressed from the source and sink perspective. The limiting data collection should be consistent with this concept.

Table 3.2.Limiting data for Example 3.2 (Polley and Polley, 2000)

SKj	F_{SKj} (ton/h)	C_{SKj} (ppm)	SRi	F_{SRi} (ton/h)	C_{SRi} (ppm)
1	50	20	1	50	50
2	100	50	2	100	100
3	80	100	3	70	150
4	70	200	4	60	250

For the first step, the water source and sink composite curves should be plotted on water flow rate (x-axis) versus impurity load (y-axis) diagram from the origin. In order to do this, the cumulative mass load (Cum. Δm) and cumulative flow rate (Cum. F) of sources and sinks are calculated as demonstrated in Table 3.3.

Table 3.3.Calculate cumulative flow rate and mass loads for Example 3.2

1	2	3	4	5	6
SKj	C_{SKj} (ppm)	F_{SKj} (ton/h)	Δm_{SKj} (kg/h)	Cum. F_{SKj} (ton/h)	Cum. Δm_{SKj} (kg/h)
1	20	50	1	50	1
2	50	100	5	150	6
3	100	80	8	230	14
4	200	70	14	300	28
SRi	C_{SRi} (ppm)	F_{SRi} (ton/h)	Δm_{SRi} (kg/h)	Cum. F_{SRi} (ton/h)	Cum. Δm_{SRi} (kg/h)
1	50	50	2.5	50	2.5
2	100	100	10	150	12.5
3	150	70	10.5	220	23
4	250	60	15	280	38

First of all, contaminant concentrations of sources and sinks are arranged in increasing order and presented with their respective flow rates in column 2 and 3. Multiplying flow rates and contaminant concentrations, the mass loads for sinks and sources are determined in column 4. Cumulative flow rate (column 5) and mass load (column 6) are identified by cascading down the flow rates and mass loads, respectively. Then, plotting column 5 versus column 6 in x-y diagram, the sink and source composite curves can be readily formed as shown in Figure 3.4.

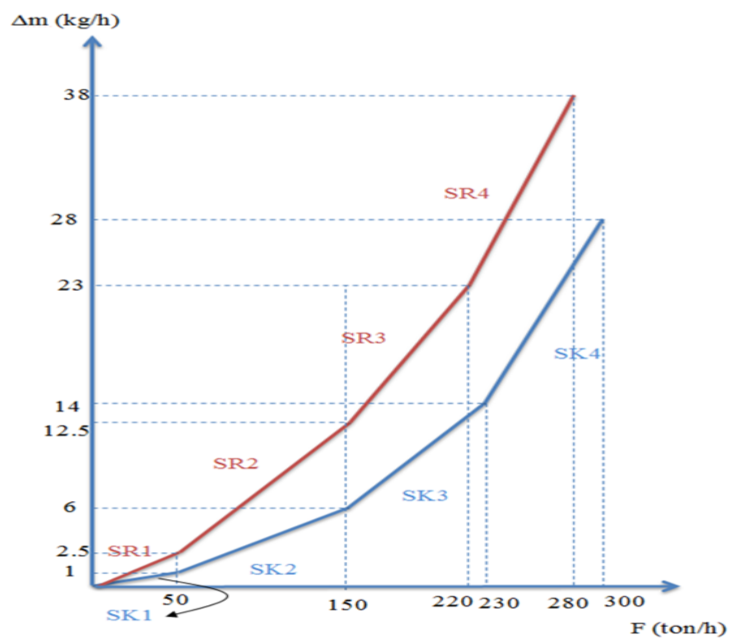

Figure 3.4.Source and sink composite curves in MRPD method

Considering the feasibility constraint implies that at any given impurity loads (turning points) the flow rate of each source should be equal or more than that of every sink. Hence, for targeting minimum freshwater (F_{fw}) and wastewater (F_{ww}) flow rate, source composite curve should be shifted horizontally until it entirely locates below and the right side of sink composite curve with intercept at the pinch point (Figure 3.5). Pinch point divides the total system into the higher quality region (below the pinch concentration) and lower quality region (above the pinch point). Among all of processes sources and sinks, only the pinch causing source (SR3) allocates to the both regions. The overlap between source and sink composite curve identifies the maximum opportunity of water recovery considering reuse/recycle scheme. Furthermore, the overhang below and above the pinch point corresponds to the minimum freshwater (70 to/h) and wastewater

(50 ton/h) flow rate targets, respectively. The original network requires 300 ton/h of freshwater and disposed 280 to/h of waste. Maximum of 76% freshwater saving and 82% of waste water reduction are possible with reuse/recycle scenario.

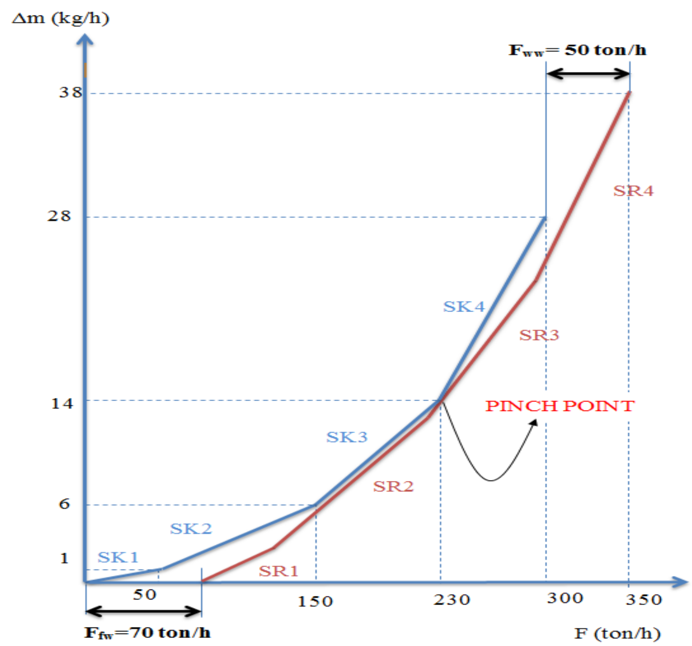

Figure 3.5.Pinched composite curves for MRPD method

Alwi and Manan (2007) later extended this targeting technique to address multiple utilities problem. Two water sources, one pure freshwater and the other with 80 ppm contaminant concentration, are assumed in Figure 3.6. Since the impure utility's contaminant concentration is higher than SR1, the impure utility locus is connected to the end of SR1 without considering the rest of process sources. These two segments are moved horizontally to touch the sink composite curve at the utility pinch point. The overhang on the left end targets the minimum pure freshwater demand (56.25 ton/h). The reaming processes sources are arranged in the increasing order of contaminant concentration to form the source composite curve for SR2 to SR4. This composite curve is slid on the impure freshwater locus until another pinch point is created. The minimum flow rate for impure utility is given by the horizontal distance of impure fresh water locus

(43.75 ton/h) while the gap between composite curves on the right end targets the minimum wastewater generation (80 ton/h).

In comparison with the single pure freshwater case, the demand for pure freshwater is decreased by 19%, however, the wastewater flow rate rises by 38%. Hence, the economic optimality is not guaranteed. The trade-off between freshwater supply cost and the expense for wastewater treatment facilities should be studied.

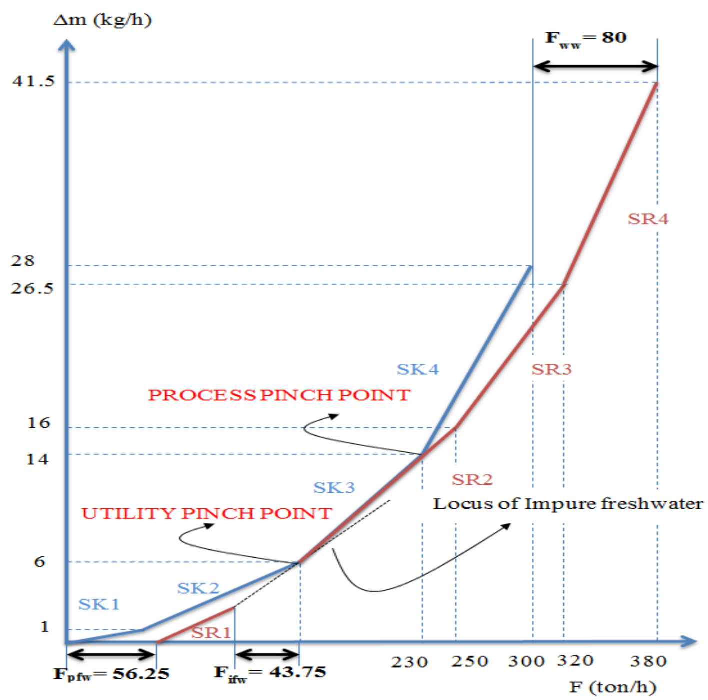

Figure 3.6.Targeting multiple utilities problem using MRPD method

The MRPD also gives engineers an insight for regeneration unit placement. The pinch point separates the total network to two regions: the region with the deficiency of process sources (below the pinch) and the surplus region (above the pinch) (El-Halwagi, 2006). This observation can be utilised to locate the regeneration unit across the pinch concentration, that is, some amount of flow rate for process source in surplus region is partially purified and recycled back to the sinks located below the pinch. In this way, both freshwater and wastewater flow rates are reduced.

The main limitation of this method is the visual resolution. It is not very easy to locate the pinch point(s) where the slope of sources and sinks segments are close or having similar values. For these cases, the magnification of graphical presentation around the pinch point is required. From this aspect, Water Cascade Analysis (WCA) as an algebraic targeting tool can better deal with such limitations and is described in the following section.

3.1.3 Water Cascade Analysis

The general procedure of WCA method is illustrated by water cascade tables (Table 3.4 & Table 3.5) for flow rate targeting in the water network synthesis (Manan et al., 2004). Example 3.2 is revisited to help with the explanation of this technique.

1) The concentrations of all process sources and sinks are grouped and arranged in the increasing order and shown with the summed up respective flow rates in the first four columns. Please note that, the maximum possible contaminant concentration (1 million ppm) is also added at the bottom of the second column.
2) Then, the sum of the flow rate of the process sinks subtracted from the sum of the flow rate of the process sources at every impurity level gives the net flow rate in column 5.
3) The net flow rate is cascaded down to obtain the cumulative flow rate ($F_{c,k}$) in column 6. The first entry indicates the fresh water flow rate. However, it is assumed to be zero at this step (Table 3.4) and will be modified later (Table 3.5).
4) The interval impurity loads (Δm_k) are determined in column 7. These values are calculated by multiplying the cumulative flow rate (column 5, $F_{c,k}$) with the difference of contaminant concentration across each interval (column 2, C_{k+1}-C_k), where $F_{c,k}$ is located.
5) Assuming the zero impurity load as the first entry in column 8, the interval impurity load is cascaded down which yields the cumulative load (*Cum.* Δm_k). If negative values are observed in column 8, the interval fresh water flow rates ($F_{\mathrm{fw},k}$) for every impurity level are calculated using Eq 3.2 and

inserted in column 9. C_{fw}, contaminant concentration for freshwater source, sets be zero due to the pure water feed assumption.

$$F_{fw,k} = \frac{cum.\Delta m_k}{(C_k - C_{fw})} \tag{3.2}$$

Table 3.4.The infeasible water cascade table

1	2	3	4	5	6	7	8	9
k	C_k (ppm)	S.F_{SKj} (ton/h)	S.F_{SRi} (ton/h)	S.F_{SRi}- S.F_{SKj} (ton/h)	$F_{c,k}$ (ton/h)	Δm_k (kg/h)	Cum. Δm_k (kg/h)	$F_{fw,k}$ (ton/h)
					F_{fw}=0			
1	0			0				
					0	0		
2	20	50		-50			0	0
					-50	-1.5		
3	50	100	50	-50			-1.5	-30
					-100	-5		
4	100	80	100	20			-6.5	-65
					-80	-4		
5	150		70	70			-10.5	-70
					-10	-0.5		
6	200	70		-70			-11	-55
					-80	-4		
7	250		60	60			-15	-60
					-20	-19995		
8	10^6						-20010	-20

6) Finally, the absolute value of the largest negative in column 9 (70 ton/h) identifies the minimum fresh water flow rate target. This value replaces the pre-assumed fresh water flow (zero flow rate) in the first entry of column 5.
7) The pre-described procedure is repeated until all negative values in column 8 are eliminated and the feasible water cascade table (Table 3.5) is thus constructed without the 9th column of infeasible water cascade table. The last entry in column 6 shows the minimum wastewater flow rate target (50 ton/h). Furthermore, the zero cumulative mass load is associated with pinch concentration in column 2 (150 ppm).

The additional target reported via this method is the flow rate allocation of pinch causing source to higher and lower concentration region which is found in the 6th column of Table 3.5 across the pinch point. While 10 ton/h of SR3 is assigned for higher quality region, 60 ton/h is for higher concentration (lower quality) region.

Table 3.5.The feasible water cascade table for targeting single pure fresh water scenario

1	2	3	4	5	6	7	8
k	C_k (ppm)	S.F_{SKj} (ton/h)	S.F_{SRi} (ton/h)	S.F_{SRi}- S.F_{SKj} (ton/h)	$F_{c,k}$ (ton/h)	Δm_k (kg/h)	Cum. Δm_k (kg/h)
					F_{fw}=70		
1	0			0			
					70	1.4	
2	20	50		-50			1.4
					20	0.6	
3	50	100	50	-50			2.0
					-30	-1.5	
4	100	80	100	20			0.5
					-10	-0.5	
5	150		70	70			0
					60	3.0	
6	200	70		-70			3.0
					-10	-0.5	
7	250		60	60			2.5
					F_{ww}=50	49987.5	
8	10^6						49990

The modified procedure of WCA has been proposed for the presence of multiple utilities with different concentrations (Foo, 2007). A three-step approach to target the minimum flow rate for each utility is put forward:

- Identify the flow rate for the lower quality water source;
- Determine the flow rate for the higher quality water source;
- Adjust the flow rate for the lower quality water source.

The basic principle underlying these three steps is the generic WCA discussed earlier. One can refer to references (Foo, 2007, 2012) for more detailed description.

Applying WCA (Foo et al., 2006; Manan et al., 2004), regeneration water network can be targeted under the guideline of Hallale (2002). The method was further enhanced to target all the key parameters in regeneration problem based on the concept of flow rate relocation between freshwater and regenerated water region (Ng et al., 2007b, 2008). Although, WCA is a promising tool, the solving procedure is iterative. Moreover, it does not give a conceptual view because of its pure algebraic characteristic. It has not been applied for the inclusion of removal ratio type regenerator.

The Composite Table Algorithm is a combined graphical and numerical targeting method. . It gives not only the physical insight but also the numerical accuracy for the problem. Therefore, it somehow overcomes the disadvantages of MRPD and WCA and will be introduced in the following section.

3.1.4 Composite Table Algorithm

Composite Table Algorithm (CTA) (Agrawal and Shenoy, 2006) is the extension of Mass Problem Table (Castro et al., 1999) to handle FF problems. Although CTA is conceptually similar to WCA, its application is easier. To utilize CTA, it is not necessary to consider both water cascade and pure water surplus cascade diagrams. Therefore, the steps required to achieve targets are less than WCA.

Revisiting Example 3.2, the implementation of CTA is demonstrated in Table 3.6 and the sequential procedure is described:

Table 3.6.Implementation of CTA

SK1	SK2	SK3	SK4	SR1	SR2	SR3	SR4	1	2	3	4	5	6
50	100	80	70	50	100	70	60	k	C_k (ppm)	Net.F_k (ton/h)	Δm_k (kg/h)	Cum.Δm_k (kg/h)	$F_{fw,k}$ (ton/h)
								1	20			0	0
										50	1.5		
								2	50			1.5	30
										100	5		
								3	100			6.5	65
										80	4		
								4	150			10.5	70
										10	0.5		
								5	200			11	55
										80	4		
								6	250			15	60
										20	(1)		
								7	(300)			(16)	(53.33)

1) Column 2- The concentrations (C_k; k=1, 2,…NC) of process sinks and sources, grouped and arranged in an increasing order. One arbitrary value (larger than others) is added in the last cell (300 ppm for this example).

2) Column 3 - The interval net flow rate (Net.F_k): For each concentration interval (C_{k+1}, C_k), the sum of source flow rates is subtracted from the sum of sink flow rates. The streams are represented by vertical arrows with the flow rates indicated at the title row. Every arrow starts with a limiting concentration and ends on the largest arbitrary concentration. In this way of presentation, the stream population of process sources and sinks can be easily observed. It is worth mentioning that the last value of this column determines the total system flow rate loss/gain. If the value is positive, the total system encounters water loss and vice versa. For this example, the total flow rate loss is calculated to be 20 ton/h.

3) Column 4 - The interval impurity loads (Δm_k): These values are calculated by multiplying the interval net flow rate (Net.F_k) with the difference of contaminant concentration levels (C_{k+1}-C_k), where Net.F_k is located.

4) Column 5 - The cumulative load (Cum. Δm_k): By assuming the zero impurity load as the first entry, the interval impurity load (Δm_k) is cascaded down to generate the cumulative load.

5) Column 6 - The interval freshwater flow rate for reuse/recycle scheme ($F_{fw,k}$) calculated via Eq 3.2. Note that due to the assumption of pure freshwater supply, contaminant concentration of freshwater (C_{fw}) is set to be zero. The largest value of this column is the required minimum pure freshwater flow rate target (70 ton/h) and its corresponding concentration level is the pinch concentration (150 ppm) for the reuse/recycle network.

6) The wastewater flow rate and its contaminant concentration can be calculated by applying flow rate (Eq 3.3) and mass balances (Eq 3.4) over the total system:

$$F_{fw} - F_{ww} = \sum_j F_j - \sum_i F_i \qquad (3.3)$$

$$F_{fw} \times C_{fw} - F_{ww} \times C_{ww} = \sum_j F_j C_j - \sum_i F_i C_i \qquad (3.4)$$

Note that the right side of Eq 3.3 is the total amount of flow rate loss/gain calculated in step 2 of CTA. In this example, the loss is 20 ton/h and F_{fw} = 70 ton/h, therefore, the wastewater flow rate is 50 ton/h. From Eq. 3.4, the wastewater contaminant concentration (C_{ww}) is obtained as 200 ppm.

Plotting column 2 versus column 5 of Table 3.6 in y-x diagram forms the graphical presentation of CTA (Figure 3.7). The inverse slope of water supply line targets the minimum fresh water demand for the network. Since the results are identical, the hybrid graphical and numerical characteristic of CTA can be concluded.

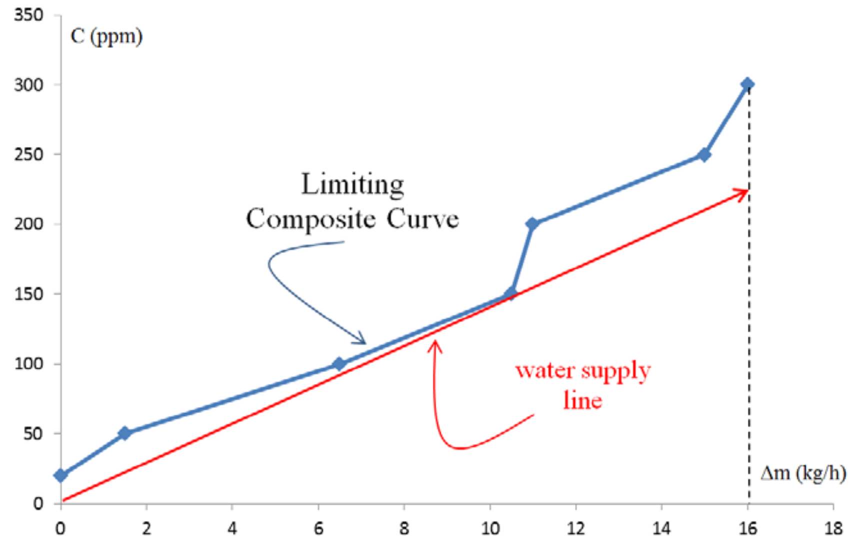

Figure 3.7.Graphical presentation of CTA

This figure shows a similar graphical characteristic with that obtained by Limiting Composite Curve (LCC) method. Nevertheless, CTA is implementable for FF problem while LCC can only be used for FL problems.

As described earlier, because LCC sets the constraint for mass load transfer, the use of CTA for multiple utilities problem can be readily addressed (Deng and Feng, 2011). The idea is to pinpoint the utility concentration on the LCC and adjust water supply line accordingly; the minimum freshwater flow rate can then be targeted for all utilities serving the network. This approach was also utilised for the simultaneous inclusion of multiple utilities and regeneration unit for the first time as well as the placement of pre-treatment system.

The data provided by CTA can further be used for the targeting of total water regeneration and regeneration-recycle network (Agrawal and Shenoy, 2006; Agrawal and Shenoy, 2007; Liao et al., 2007). LCC was formed from the results of performing CTA. Then based on this graphical presentation, the targets for the regeneration–reuse/recycle water network are established. However, in dealing with highly integrated water networks, the above proposed technique is not completely reliable to set the targets. The interpretation of the graphical presentation can be very tedious when the turning points of LCC are not clearly distinguishable. The same limitation also exists for the zero liquid discharge special case.

In conclusion, although CTA is completely hybrid in graphical and numerical for reuse/recycle water network, this argument would not be held correctly for regeneration problems. Thus, the extension of CTA's numerical step for targeting regeneration water network is valuable.

3.2 Network design

Applying pinch analysis to water network synthesis, two sequent stages, targeting and design, are normally adopted. So far, it has been demonstrated how the minimum utilities targets could be identified prior to the network design for various water network problems. Through this section, two water pinch network design methods, Nearest Neighbor Algorithm (NNA) and Three Design Rules (TDR), are introduced. Whilst the former is suitable for FF problems, the latter could handle FL operations.

3.2.1 Nearest Neighbor Algorithm

The principal of nearest neighbour can be briefly stated as: to fulfil the particular demand, two nearest neighbor in term of contaminant concentration should be selected. In other words, the sources which are just cleaner and dirtier than the specific sink are mixed together to satisfy this process sink. Satisfying the process demand, two criteria should be met i.e. flow rate and mass load. To address both of these requirements in the network design, the following steps of NNA are proposed by Prakash and Shenoy (2005b):

1) Arrange all process sinks and sources in ascending order of contaminant concentration. Note that sources should comprise the regenerated sources and external freshwater sources (if any). Start the design for the highest quality process sink.
2) If the source exists with the same concentration of process sink, match them together.
3) Mix two nearest neighbor sources to the sink to be satisfied. Designating sources, SR_i (with flow rate of F_{SRi} and contaminant concentration of C_{SRi}) and SR_{i+1} (with flow rate of F_{SRi+1} and contaminant concentration of C_{SRi+1}), and the sink, SK_j where C_{SKj} is just higher than C_{SRi} and lower than C_{SRi+1} ($C_{SRi} < C_{SKj} < C_{SRi+1}$), the allocated flow rates between sources and sink are deduced via the flow rate balance (Eq 3.5), and the mass balance (Eq 3.6).

$$F_{SKj} = F_{SRi,SKj} + F_{SRi+1,SKj} \qquad (3.5)$$

$$F_{SKj} \times C_{SKj} = F_{SRi,SKj} \times C_{SRi} + F_{SRi+1,SKj} \times C_{SRi+1} \qquad (3.6)$$

4) If the allocated flow rate is greater than the available source flow rate, for instance $F_{SRi,SKj} > F_{SRi}$, the entire candidate source (*SRi)* is exhausted. Then, the new pair of nearest neighbor sources is considered to satisfy the sink.
5) Steps 2 to 4 are repeated until all sinks are satisfied.

To explain this design procedure further, revisit Example 3.2 with limiting data provided in Table 3.2. The targets were established using MRPD/WCA/CTA for the minimum freshwater (70 ton/h), wastewater (50ton/h, 200 ppm), and pinch (150 ppm). The convenient presentation of network design applying NNA is matching matrix (Figure 3.8). While the sources are arranged as rows, the sinks are organized as columns in the ascending order of contaminant concentrations. Note that fresh water (FW) should be considered as one of the sources and it is the first entry column of matching matrix.

		F_{SKj} (ton/h)	50	100	80	70	50
		C_{SKj} (ppm)	20	50	100	200	200
F_{SRi} (ton/h)	C_{SRi} (ppm)	SK_j / SR_i	SK1	SK2	SK3	SK4	WW
70	0	FW	30	35	5		
50	50	SR1	20	30			
100	100	SR2		35	65		
70	150	SR3			10	35	25
60	250	SR4				35	25

Figure 3.8.Network design as a matching matrix for example 3.2

Network design starts for the highest quality sink (SK1) with 20 ppm contaminant concentration. Since there is no source with the same contaminant concentration, two nearest neighbor sources, FW (0 ppm) and SR1 (50 ppm), are chosen to satisfy SK1. Eqs 3.5 and 3.6 give $F_{FW,SK1}+F_{SR1,SK1} = 50$ and $F_{FW,SK1}(0) + F_{SR1,SK1}(50) = 50(20)$ which are solved to obtain $F_{FW,SK1} = 30$ ton/h and $F_{SR1,SK1} = 20$ ton/h. Both allocated flow rates are less than available amount. Hence, SK1 is completely satisfied by FW and SR1. The flow rates of FW and SR1 are updated as 40 ton/h and 30 ton/h respectively.

The next cleanest sink is SK2 with 50 ppm contaminant concentration. SR1 (30 ton/h, 50 ppm) is completely exhausted ($F_{SR1,SK2}$= 30 ton/h). However, SK1 is not completely satisfied yet. The nearest neighbor sources are FW (40 ton/h, 0 ppm) and SR2 (100 ton/h, 100 ppm). Applying Eqs. 3.5 and 3.6 give $F_{FW,SK2}$ = 35 ton/h and $F_{SR2,SK2}$ = 35 ton/h. Since both of flow rate allocations are less than available amounts, SK2 is entirely satisfied.

To satisfy SK3, 65 ton/h of SR2 with same quality (100 ppm) is available. The remaining requirement is fulfilled by two available nearest neighbor sources, FW, and SR3. The same as before, the flow rate allocations are calculated as $F_{FW,SK3}$ = 5 ton/h, and $F_{SR3,SK3}$ = 10 ton/h. All the below pinch sources including freshwater are completely utilised by this stage.

SR3 is the pinch-causing source which can be allocated to both regions (below and above pinch). The shaded cells are the indication of forbidden matches across the pinch. SK4 located in the lower quality region (above pinch) is satisfied by nearest neighbor sources (SR3 and SR4). The flow rate allocation are calculated as $F_{SR3,SK4}$ = 35 ton/h and $F_{SR4,SK4}$ = 35 ton/h. All of the process sinks are completely fulfilled and the remaining flow rate of SR3 (25 ton/h) and SR4 (25 ton/h) are wastewater streams.

Following the aforementioned procedure, the allocated flow rate are calculated and inserted into the corresponding cells in the matching matrix. This matching matrix demonstrates that all the targets can be achieved in practice through the network design.

The NNA is also applicable for multiple utilities (Shenoy and Bandyopadhyay, 2007) and regeneration (Agrawal and Shenoy, 2006) problems. For the former problems, all utilities with the targeted flow rate are arranged within the sources, and then implementing the rules of NNA forms the network. For the regeneration problems, the outlet and inlet regeneration streams are considered as one of the process sources and sinks, respectively. Since the regenerated water flow rate is also known from the targeting stage, applying NNA step by step can produce the process flow sheet.

Applying NNA for FL problems, the targets can be met. Nevertheless, firstly, the network is relatively complex; secondly, the water flow rate passing every operation is relatively high which causes higher capital cost.

3.2.2 Three Design Rules

To address both of above-mentioned deficiencies of NNA, Three Design Rules (TRD) were developed by the same researcher (Prakash and Shenoy, 2005b) to design the network including FL processes. These rules are as follows:

Rule 1: All units should have their maximum allowable outlet concentrations.

Rule 2: If the operations cross the pinch, the inlet concentration must be forced to the maximum allowable value. This rule can be easily carried out by NNA.

Rule 3: If the water-using processes are completely below or above the pinch, the cleanest available source is used to the maximum amount to satisfy these processes. Note that no sources from below the pinch should be used to satisfy the processes above the pinch and vice versa.

To explain these criteria further, revisit Example 3.1 with the limiting data listed in Table 3.1. According to pre-specified targets, this network requires 90 ton/h of pure freshwater; it generated 90 ton/h of wastewater with contaminant concentration of 455.6, and the pinch concentration is 100 ppm considering the reuse/recycle scheme. The network is designed using TDR and the relevant water flow sheet is depicted in Figure 3.9.

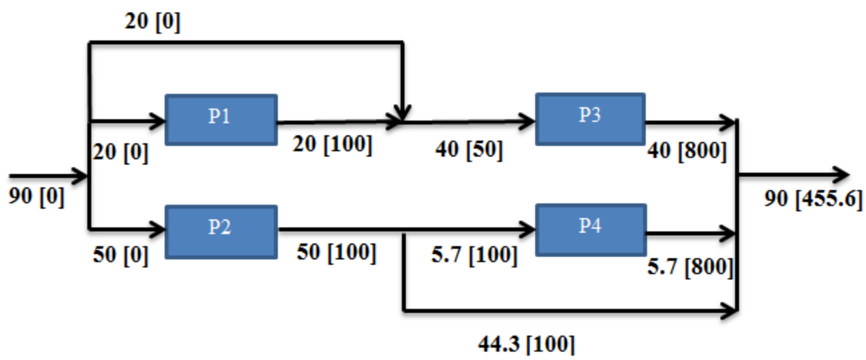

Figure 3.9.Network design for example 3.1 (Numbers in [ ] are contaminant concentrations in ppm and outside [ ] are flow rates in ton/h)

P1 and P2 are the below pinch processes. The design begins with the most stringent process (P1) and continues in the ascending order of contaminant concentration. As per Rule 3, the cleanest source (pure freshwater) should be used to the maximum extent at meantime, Rule 1 also should be met. The freshwater requirement for P1 is calculated via Eq 3.1 (2000/(100-0)) as 20 ton/h. By now, the available sources are the freshwater (70 ton/h, 0 ppm), and outlet P1 stream (20 ton/h, 100 ppm). According to Rule 3, P2 needs 50 ton/h of freshwater to be satisfied.

P3 is an across-pinch operation with the maximum inlet concentration (50 ppm) below the pinch (100 ppm) and the maximum outlet concentration (800 ppm) above the pinch. By this stage, 20 ton/h of freshwater, outlet stream of P1 (20 ton/h, 100 ppm), and P2 outlet stream (50 ton/h, 100 ppm) could be utilised to satisfy P3. The nearest neighbor sources are freshwater source (0 ppm) and either of P1 or P2 with 100 ppm contaminant concentration. Here, the freshwater and P1 outlet stream are chosen to be fed into P3. Based on Rule 2, the required flow rate for each source can be calculated via Eqs 3.5 and 3.6 ($F_{FW,P3}+F_{P1,P3} = 40$ & $F_{FW,P3}(0)+F_{P1,P3}(100) = 40(50)$) . All of the available freshwater (20 ton/h) and P1 outlet stream (20 ton/h) sources are exhausted to pick up the impurity load of P3.

P4 is an above pinch unit and the outlet of P2 (50 ton/h, 100 ppm) is the cleanest available source. 5.7 ton/h of P2 outlet steam is reused in P4 while the rest of amount (44.3 ton/h) disposed to the environment. Thus, all the processes are satisfied.

3.3 Summary

In this chapter, some of water pinch targeting and design methods are chosen to be discussed in detail. These methods provide a fundamental knowledge to make the rest of thesis comprehensible. The basic information of CTA is in need to understand Chapters 4, 5 and 6. MRPD and WCA are going to be utilised in Chapter 7. The network design methods will be employed to construct the process flow sheet in each chapter depending on the type of problem.

4. COMPOSITE TABLE ALGORITHM FOR VARIOUS PROBLEMS IN REUSE/RECYCLE WATER NETWORK

The Composite Table Algorithm (CTA) has been used for water reuse/recycle network, regeneration reuse/recycle problem (Agrawal and Shenoy, 2006), zero liquid discharge network (Deng et al., 2008), and multiple utilities problem (Deng and Feng, 2011) considering Fixed Flow rate (FF) operations. CTA has several advantages compared to other existing targeting methods. These advantages are highlighted as follows:

- It is more analogous to seminal pinch targeting technique proposed by Wang and Smith (1994b). Hence, CTA can easily be extended to cope with various water network synthesis problems.
- It is the combination of graphical and numerical targeting technique, therefore, provides numerical accuracy as well as physical insight.
- It requires less calculation effort in terms of numerical analysis.
- Due to these reasons, extension of this technique to be capable of addressing various problems in water network synthesis is worthwhile. It is believed that CTA can become one of the well-established targeting techniques.

In this chapter, the further possible applications of CTA can be seen in Fixed Load (FL) problem as well as hybrid problem with combined FL and FF operations. Moreover, the applicability of this method for threshold and multiple pinches problems is also studied. To facilitate the implementation, the approach has been programed in MATLAB. The steps of CTA and its applicability to deal with FF problems can be found in Chapter 3, if refreshment of knowledge is necessary.

4.1 Problem statement

The superstructure presentation of the problem is depicted in Figure 4.1.

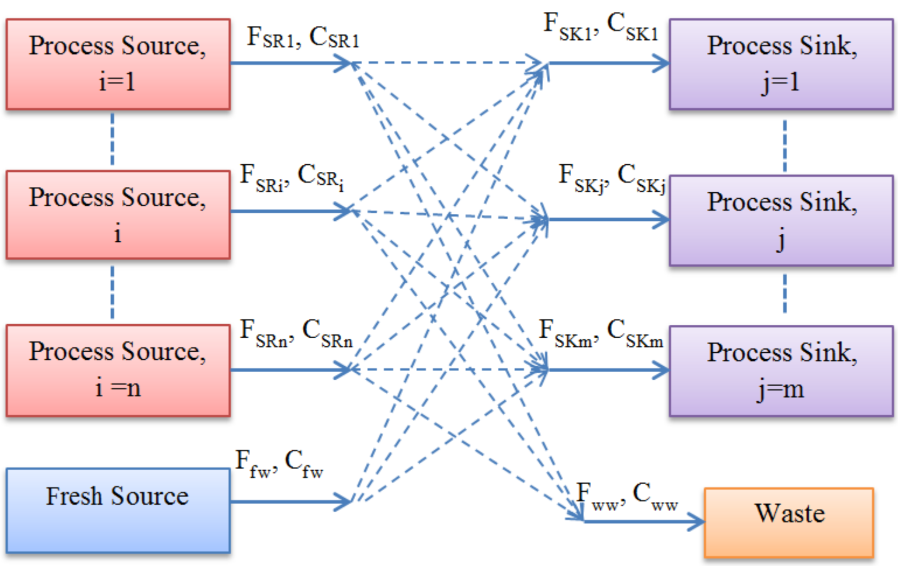

Figure 4.1.Sources/Sinks superstructure presentation for reuse/recycle water network

Consider a process that includes set of process sinks and set of process sources:

- Processes needing water are designated as Process Sinks or SKj (j=1, 2, … *m*). Each sink has a given flow rate, F_{SK_j} and inlet concentration, C_{SKj}, which must satisfy: $C_{SKj}{}^{min} \leq C_{SKj} \leq C_{SKj}{}^{max}$, where $C_{SKj}{}^{min}$ and $C_{SKj}{}^{max}$, is the lowest and the highest of concentration limit.
- Water-generating processes, which are reused or recycled to Process Sinks are designated as Process Source, or SRi (i= 1, 2,…, *n*), with a given flow rate of F_{SRi}, and an impurity concentration of C_{SRi}.
- If Process Sources cannot satisfy Process Sinks, an external pure freshwater source (C_{fw} = 0) with flow rate of F_{fw} is introduced to fulfil the requirement of the sinks flow rate. Unused water from process sources (if any) will be directed to the waste with the concentration of (C_{ww}) and the flow rate of (F_{ww}).

Given the above-described process, the objective is to find the targets, freshwater (F_{fw}) and wastewater (F_{ww}) flow rates, for various water network problems including FL, combined FL and FF, multiple pinch, and threshold considering reuse/recycle scheme. Having set up the targets, the water allocation network is constructed for every problem.

4.2 Fixed Load operations

As mentioned in preceding chapters, FL water network comprises processes which are quality controlled such as, washing, scrubbing, etc. The main concern for these types of operation is the amount of contaminant mass removal. In this model, each operation has maximum allowable inlet (C_{in}) and outlet (C_{out}) contaminant concentrations specified by the process constraints. The main assumption is that the water flow rate (F) keeps as constant throughout the process. Then, the fixed amount of mass load (M) will be picked up by water via Eq 4.1.

$$M = F(C_{out} - C_{in}) \qquad (4.1)$$

Consider Example 4.1 adopted from Wang and Smith (1994b). This example was analysed in previous chapter using LCC to find the targets. Later, this problem was targeted by WCA (Manan et al., 2004) and MRPD (Prakash and Shenoy, 2005b) methodologies. This is a typical FL problem and the limiting data is again listed in Table 4.1.

Table 4.1.Limiting data for Example 4.1 (Wang and Smith, 1994b)

Process, P_p	Δm_p (kg/h)	C_{in} (ppm)	C_{out} (ppm)	F_p (ton/h)
1	2	0	100	20
2	5	50	100	100
3	30	50	800	40
4	4	400	800	10

To utilise the CTA for FL problems, for the first step, it is essential to convert the limiting data from FL problem to source/sink perspective. To do so, as described earlier in Chapter 2, an inlet stream to any process should be considered as a sink and an outlet stream from any operation is treated as a source. The converted limiting data are shown in Table 4.2.

Table 4.2.Converted limiting data to FF model for Example 4.1

Sink	F_{SKj} (ton/h)	C_{SKj} (ppm)	Source	F_{SRi} (ton/h)	C_{SRi} (ppm)
$P1_{in}$	20	0	$P1_{out}$	20	100
$P2_{in}$	100	50	$P2_{out}$	100	100
$P3_{in}$	40	50	$P3_{out}$	40	800
$P4_{in}$	10	400	$P4_{out}$	10	800
Total	170		Total	170	

The next step is to implement CTA as described in Chapter 3 and the results are shown in Table 4.3. Here, the stream population of process sources and sinks is excluded. The minimum freshwater flow rate target is found as 90 ton/h and the pinch point locates at 100 ppm contaminant concentration. The last entry in the third column (Net.F_k), which determines the total flow rate loss/gain of the network, equates to zero. This observation means that all the involved operations in the network are FL processes.

Table 4.3.Implementation of CTA for Example 4.1

k	C_k (ppm)	Net.F_k (ton/h)	Δm_k (kg/h)	Cum.Δm_k (kg/h)	$F_{fw,k}$ (ton/h)
1	0			0	0
2	50	20	1	1	20
3	$\underline{100}$	160	8	9	$\underline{90}$
4	400	40	12	21	52.5
5	800	50	20	41	51.25
6	(850)	0	(0)	(41)	(48.23)

The LCC created by MATLAB (Blue line) is illustrated in Figure 4.2. The last segment of LCC whose inverse slope is zero presents the amount of water loss/gain. Furthermore, the end point of water supply line (red line) corresponds to the wastewater contaminant concentration (C_{ww}) to be 455.6 ppm. Therefore, there is no more need for additional calculation to find C_{ww}. However, this argument is only acceptable for FL problems which could be recognized as a part of CTA implementation (either vertical line for the last segment of LCC, or the zero entry for the last row of Net.F_k column)

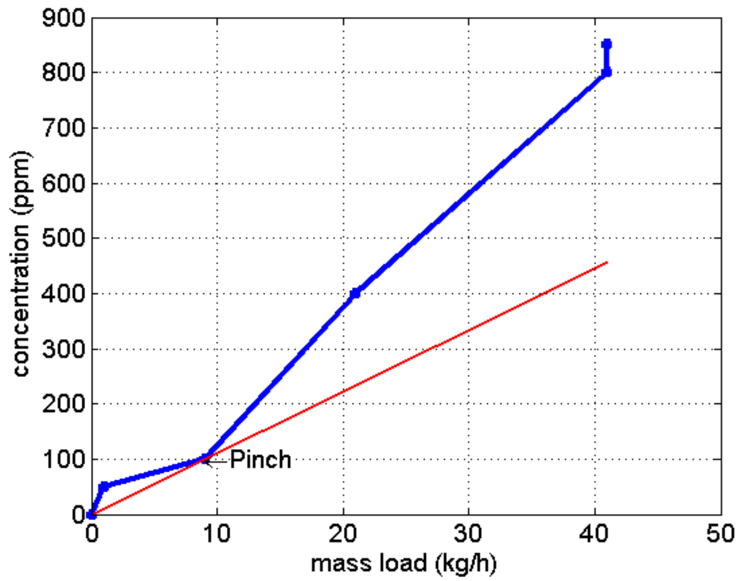

Figure 4.2.The graphical of CTA for Example 4.1

Thus, it has been demonstrated that the CTA, originally developed for FF problems, also can handle FL water network if the data transformation is correctly performed. One possible network design satisfying all targets was presented by Figure 3.9 in the previous chapter.

4.3 Combined Fixed Load and Fixed Flow rate operations

To make a case of combined FF and FL operation, the data of Examples 3.2 and 4.1 are merged to form the new limiting data (Table 4.4). The same example was addressed by Prakash and Shenoy (2005b) using MRPD. To implement the CTA, one should follow the same procedure outlined in Chapter 3. In this chapter, from now on, only the final targeting results with the graphical presentation of CTA are given (Table 4.4 and Figure 4.3).

To design the network, since the hybrid operations are included, the recently developed design methodology, Enhanced Nearest Neighbor Algorithm, is employed (Shenoy, 2012). In this method, Local Recycle (LR) priorities are given to FL processes and then will be eliminated by reducing the inlet contaminant concentrations.

Table 4.4.Limiting data and targeting results for Example 4.2

Limiting Data					
Sink	F_{SKj} (ton/h)	C_{SKj} (ppm)	Source	F_{SRi} (ton/h)	C_{SRi} (ppm)
$P1_{in}$	20	0	$P1_{out}$	20	100
$P2_{in}$	100	50	$P2_{out}$	100	100
$P3_{in}$	40	50	$P3_{out}$	40	800
$P4_{in}$	10	400	$P4_{out}$	10	800
SK1	50	20	SR1	50	50
SK2	100	50	SR2	100	100
SK3	80	100	SR3	70	150
SK4	70	200	SR4	60	250

Targeting Results			
F_{fw} (ton/h)	F_{ww} (ton/h)	C_{pinch} (ppm)	C_{ww} (ppm)
155	135	100	377.78

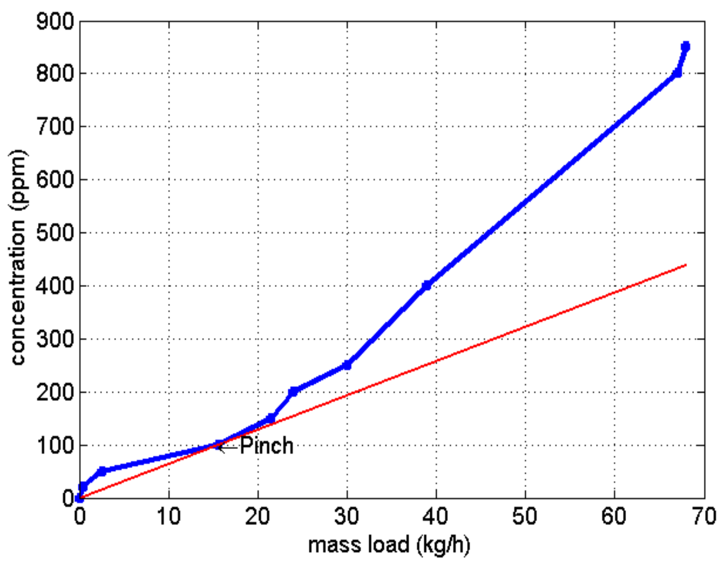

Figure 4.3.LCC and water supply line for Example 4.2

The water allocation network for Example 4.2 is depicted in Figure 4.4. The process sink, $P1_{in}$, should be satisfied by 20 ton/h of pure freshwater. Then, it is essential to consider the LR priorities for FL operations of P2, P3, and P4. The sinks (inlet streams) of these processes should be fulfilled by their sources (outlet streams) and the cleanest available source. For instance, $P2_{out}$ and FW are selected to meet the requirement of $P2_{in}$. The similar action should be done for P3 and P4.

		F_{SKj} (ton/h)	20	50	~~100~~ 50	40	100	80	70	~~10~~ 5.71	135
		C_{SKj} (ppm)	0	20	~~50~~ 0	50	50	100	200	~~400~~ 100	377.8
F_{SRi} (ton/h)	C_{SRi} (ppm)	SK_j / SR_i	$P1_{in}$	SK1	$P2_{in}$	$P3_{in}$	SK2	SK3	SK4	$P4_{in}$	WW
155	0	FW	20	30	50	5	50				
50	50	SR1		20		**30**					
20	100	$P1_{out}$				5				5.71	9.29
~~100~~ 50	100	$P2_{out}$			~~50~~ LR		**50**				
100	100	SR2						80			20
70	150	SR3							35		35
60	250	SR4							35		25
40	800	$P3_{out}$									40
~~10~~ 5.71	800	$P4_{out}$								~~4.29~~ LR	5.71

Figure 4.4.Network design for Example 4.2 as a matching matrix

As observed in Figure 4.4, although, the LR match is applicable for P4, it is forbidden cross pinch match for P3. The water allocation between sources and sinks are identified using NNA equations (Eqs 3.5 & 3.6). Then, the LR matches are omitted by adjusting the flow rates and sinks (inlet streams) contaminant concentrations via Eq 4.1. The LR eliminations and appropriate revised values are indicated within the matching matrix.

Various options exist to satisfy other process sinks. These options lead to different network design. The water allocation network presented here is just one of the possibilities. There is no more need for further description because all the remaining matches are done based on the NNA rules. All the targets are achieved through the network design. As explained for the targeting, some of sources in FF operations may satisfy the sinks in FL processes and vice versa. These matches are shown in bold through the matching matrix.

4.4 Multiple pinch problems

Multiple pinch problem is one of the classes of water network synthesis. The ability of CTA method handling this kind of problem is demonstrated through Example 4.3. The limiting data listed in Table 4.5 are taken from Sorin and Bédard (1999). The inlet and outlet flow rate for all operations except P3 are identical. This means that P3 consumes all inlet flow rate and can be considered as a flow rate loss.

Table 4.5.Limiting data for Example 4.3(Sorin and Bédard, 1999)

Process	Δm_p (kg/h)	C_{in} (ppm)	C_{out} (ppm)	F_{in} (ton/h)	F_{out} (ton/h)
P1	12	0	100	120	120
P2	7.2	50	140	80	80
P3	-	50	-	80	-
P4	5.6	140	180	140	140
P5	4.8	170	230	80	80
P6	1.95	240	250	195	195

Sources/sinks presentation of limiting data and targeting results are given in Table 4.6. Initially, only one pinch point at 180 ppm concentration was found using Evolutionary Targeting method, (Sorin and Bédard, 1999). Later several works (El-Halwagi et al., 2003; Hallale, 2002; Manan et al., 2004) have addressed this limitation.

Table 4.6.Limiting data and targeting results for Example 4.3

Limiting Data conversion					
Sink	F_{SKj} (ton/h)	C_{SKj} (ppm)	Source	F_{SRi} (ton/h)	C_{SRi} (ppm)
SK1	120	0	SR1	120	100
SK2	80	50	SR2	80	140
SK3	80	50	SR3	-	-
SK4	140	140	SR4	140	180
SK5	80	170	SR5	80	230
SK6	195	240	SR6	195	250

Targeting Results

F_{fw} (ton/h)	F_{ww} (ton/h)	$C_{pinch,1}$ (ppm)	$C_{pinch,2}$ (ppm)	C_{ww} (ppm)
200	120	100	180	299.58

In fact, CTA also has the same function as WCA, MRPD and WSD methods for multiple pinch problems. Furthermore, its non-iterative and hybrid characteristic may make it even superior to others. One also can find the relevant limiting composite curve in Figure 4.5.

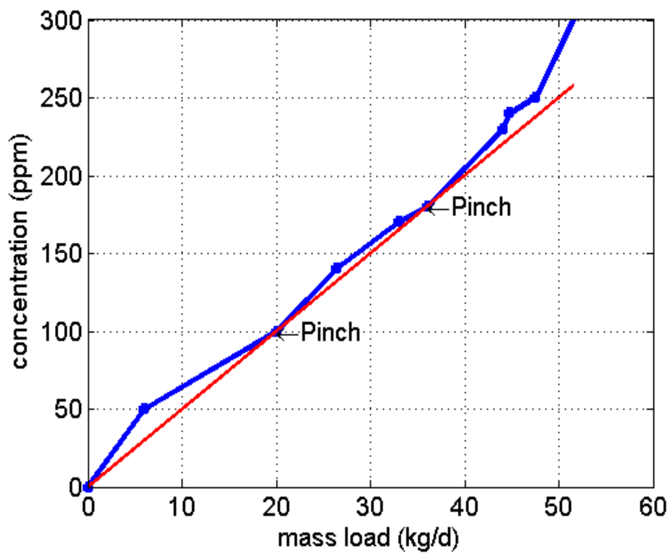

Figure 4.5.LCC and water supply line for Example 4.3

Figure 4.5 and Table 4.6 indicate that two pinch points exist for this example. Dissimilar to normal problems, these pinch concentrations divide the network to three regions: (1) the water deficit region (below the pinch concentration of 100 ppm), (2) the self-sustained region (between two pinch points), and (3) the region with the surplus of water (above the higher pinch concentration). Based on this division, P1 and P3 are located in the water deficit region, P2 and P5 are cross pinch processes, P4 is located entirely in the self-sustained region, and P6 is the above pinch process.

Three Design Rules are utilized to construct the network. Knowing the pinch points location, only P2 and P5 are satisfying using the second rule of TDR (refer back to Chapter 3) and the rest of processes should be satisfied by the cleanest available source(s) in the specified region. The process flow sheet is illustrated in Figure 4.6.

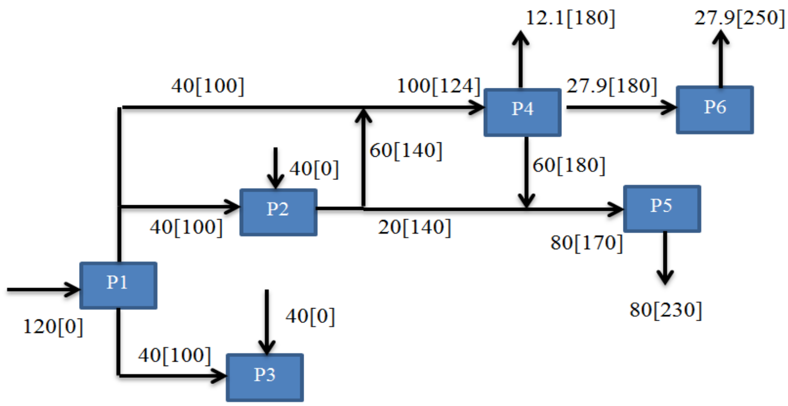

Figure 4.6.Process flow sheet for Example 4.3 (flow rates are given in t/h and concentrations are given in ppm in the parenthesis)

The water network obtained in this work is simpler than that proposed by Sorin and Bédard (1999). For instance, lower numbers of matches are found and the P6 local recycle is eliminated.

4.5 Threshold problems

Not all problems in the water network synthesis encounter fresh water consumption and waste discharge concurrently. This type of problem is termed as the "threshold problem" (Foo, 2008). In water network synthesis, the threshold problem falls in to three categories, i.e. zero network discharge with fresh water feed, network generating waste without fresh water feed, and network with no fresh water and discharge. WCA and MRPD methods have been used to address the threshold problems (Foo, 2008), we will apply CTA to achieve the same targeting. All limiting data for the following sub-sections are adopted from reference (Foo, 2008).

4.5.1 Zero freshwater supply

Limiting data listed in Table 4.7 has been selected for Example 4.4. Targeting results are also summarized in Table 4.7 and illustrated in Figure 4.7.

Table 4.7.Limiting data and targeting results for Example 4.4

Limiting Data					
Sink	F_{SKj} (ton/h)	C_{SKj} (ppm)	Source	F_{SRi} (ton/h)	C_{SRi} (ppm)
SK1	50	20	SR1	20	20
SK2	20	50	SR2	50	100
SK3	100	400	SR3	40	250
Total	170		Total	110	

Targeting Results		
F_{fw} (ton/h)	F_{ww} (ton/h)	C_{pinch} (ppm)
34	-26	100

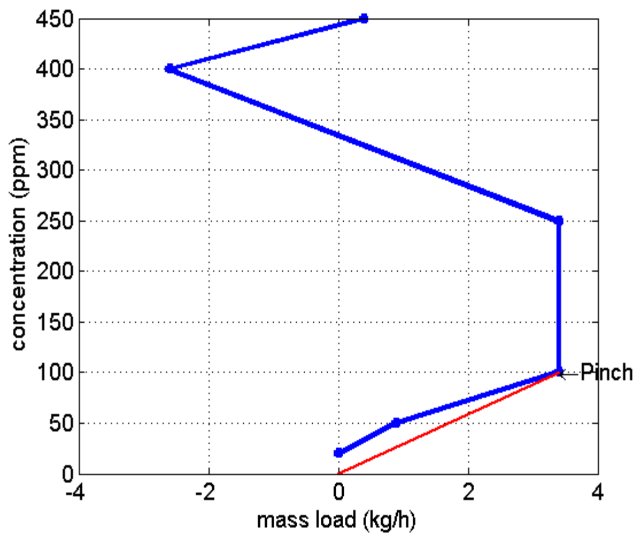

Figure 4.7.Infeasible LCC for Example 4.4

Dissimilar to previous problems, LCC section between 100-250 ppm goes vertically upward and then it directs left for 250-400 ppm concentration. This means that for the former concentration interval all sources have been reused/ recycled to process sinks thoroughly and for the latter concentration region the surplus of process sources is available. However, for the first region of LCC (between 0 and 100 ppm), fresh water is needed to fulfil the mass load constraint. The inverse slope of water supply line (shown as red) presents the amount of fresh water requirement. By inspecting the targeting results carefully, it is revealed that this amount of fresh resource is not sufficient for total system due to negative flow rate of waste water. To rectify this infeasibility, the absolute amount of waste water flow rate (F_{ww} = 26 ton/h) should be added to fresh water flow rate (F_{fw} = 34 ton/h). By doing so, the targets have changed to 60 ton/h of fresh water and 0 ton/h of waste water.

To find the pinch point, it is necessary to double check the network with the fresh water source included as one of the process resources. The fourth steps of CTA method for calculating the cumulative mass load is shown in Table 4.8. All the values for cumulative mass load are negative which means there is no more pinch point. Hence, this network consumes 60 ton/h of fresh water (64% saving) and generates zero discharge (100% saving) and no pinch point exists. These targets are completely in agreement with those reported in literature (Foo, 2008). The last concentration value (450 ppm) is known as the "threshold concentration".

Table 4.8.Feasible Cascade Table Algorithm to Find The Pinch Point For Example 4.4

C_k (ppm)	Net.F_k (ton/h)	Δm_k (kg/h)	Cum.Δm_k (kg/h)
0			0
20	-60	-1.2	-1.2
50	-30	-0.9	-2.1
100	-10	-0.5	-2.9
250	-60	-9	-11.6
400	-100	-15	-26.6
(450)	0	(0)	(-26.6)

Applying NNA, water network is synthesised as in Figure 4.8.

		F_{SKj} (ton/h)	50	20	100
		C_{SKj} (ppm)	20	50	400
F_{SRi} (ton/h)	C_{SRi} (ppm)	SK_j / SR_i	SK1	SK2	SK3
60	0	FW	24	10	26
20	20	SR1	20		
50	100	SR2	6	10	34
40	250	SR3			40

Figure 4.8.Network design for Example 4.4 as a matching matrix

Since no pinch concentration is located for this example, there is no forbidden matches region. Furthermore, to satisfy the dirtiest sink (SK3), the mass balance equation of NNA (Eq 3.6) is not taken into account.

4.5.2 Zero waste discharge

The limiting data, targeting results and LCC for Example 4.5 are listed in Table 4.9 and shown in Figure 4.9.

Table 4.9.Limiting data and targeting results for Example 4.5

Limiting Data					
Sink	F_{SKj} (ton/h)	C_{SKj} (ppm)	Source	F_{SRi} (ton/h)	C_{SRi} (ppm)
SK1	1200	120	SR1	500	100
SK2	800	105	SR2	2000	110
SK3	500	80	SR3	400	110
			SR4	300	60
Total	2500		Total	3200	

Targeting Results		
F_{fw} (g/min)	F_{ww} (g/min)	C_{pinch} (ppm)
0	700	60

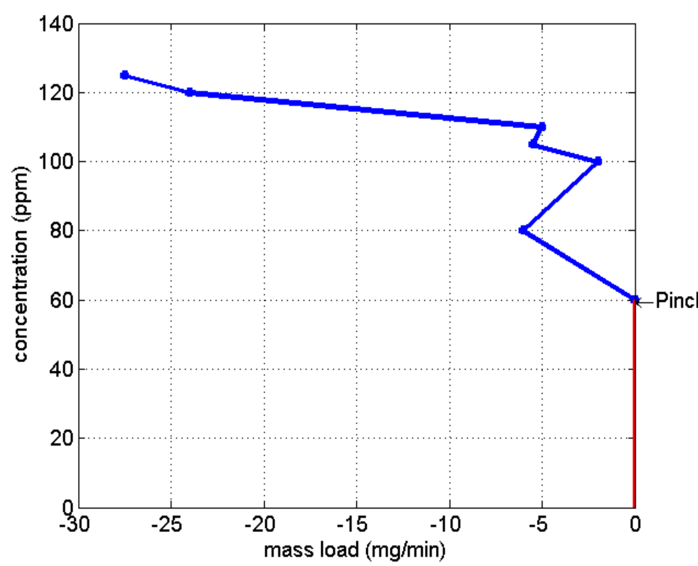

Figure 4.9.LCC and water supply line for Example 4.5

Compared to earlier examples, some uncommon characteristics of LCC need to be clarified. Firstly, LCC locates completely on the left side of mass load (negative mass load) vs. concentration diagram. This means that there is surplus of process sources to be reused or recycled to the process sinks and no fresh water is needed for total network. The vertical water supply line (in red), whose inverse slope targets the minimum fresh water requirement (0 ton/h), supports the former argument. Secondly, unlike normal problems, the trend of LCC is not always in one direction. For the segments where LCC points left, it indicates the surplus of process source for process demands within this specified concentration interval. On the other hand, LCC directing to the right means the lack of process sources for the process demands. However, for the total network, there is a surplus of water sources. These special characteristics are unique from this method and cannot easily be found via MRPD or WCA. Thirdly, the pinch point locates on the source with the lowest contaminant concentration which is uncommon for normal problems. This also means that the entire source is allocated to the lower quality region.

Targeting results have been compared with reference (Foo, 2008) for verification. Nonetheless, there is only one method involved here instead of two complementary methods used by this reference. As targeted, the network has the potential of 100% fresh water saving and reducing waste water by 2500 g/min equated to 78% after reuse/recycling takes place.

The water allocation network is depicted in Figure 4.10. Here, the cross pinch region is again does not exist because the pinch point occurs on the highest quality source. In other words, all sources and sinks belong to the lower quality region (above the pinch point). Moreover, although the flow rate requirement of lowest quality sink (SK1) is satisfied, not all the mass load is picked up. This specifically happens for the threshold problems.

		F_{SKj} (ton/h)	500	800	1200	700
		C_{SKj} (ppm)	80	105	120	
F_{SRi} (ton/h)	C_{SRi} (ppm)	SK_j / SR_i	SK3	SK2	SK1	WW
300	60	SR4	250	50		
500	100	SR1	250	250		
2000	110	SR2		500	1200	300
400	110	SR3				400

Figure 4.10.Network design for Example 4.5 as a matching matrix

It is worth mentioning that, this example is a pulp and paper industrial process originally studied by Jacob et al. (2002) using Linear Programming optimization.

The freshwater demand and wastewater generation was reported as 122 g/min and 822 g/min, respectively. As demonstrated in this study, these values are not optimum, if the objective is to minimize the freshwater requirement.

4.5.3 Zero freshwater and wastewater

Threshold problem with zero freshwater and zero discharge is rare but realistic. An organic chemical production process is adopted as the case study. This example originally was addressed by Hall (1997) with the fresh water consumption of 13 ton/h which is a sub-optimal as will be shown in this work. This case has been studied by Foo (2008) using MRPD and WCA methods.

The Limiting data, targeting results and LCC for this problem (Example 4.6) are shown in Table 4.11 and Figure 4.11, respectively. This network requires 40.5 ton/h of freshwater and generates the same amount of wastewater. Flow rate targeting results for reuse/recycle scheme reveal that, theoretically, there is potential for saving both freshwater and wastewater up to 100%.

Table 4.10.Limiting data and targeting results for Example 4.6

Limiting Data					
Sink	F_{SKj} (ton/h)	C_{SKj} (ppm)	Source	F_{SRi} (ton/h)	C_{SRi} (ppm)
Reactor	12	63	Separator	9	108
First wash	10	140	Second wash	9	70
Second wash	8	63	Column bottom	4.5	22
Stream	6.5	46	Reactor discharge	9	130
Hosepipes	4	130	Dryer	9	44
Total	40.5		Total	40.5	

Targeting Results		
F_{fw} (ton/h)	F_{ww} (ton/h)	C_{pinch} (ppm)
0	0	22

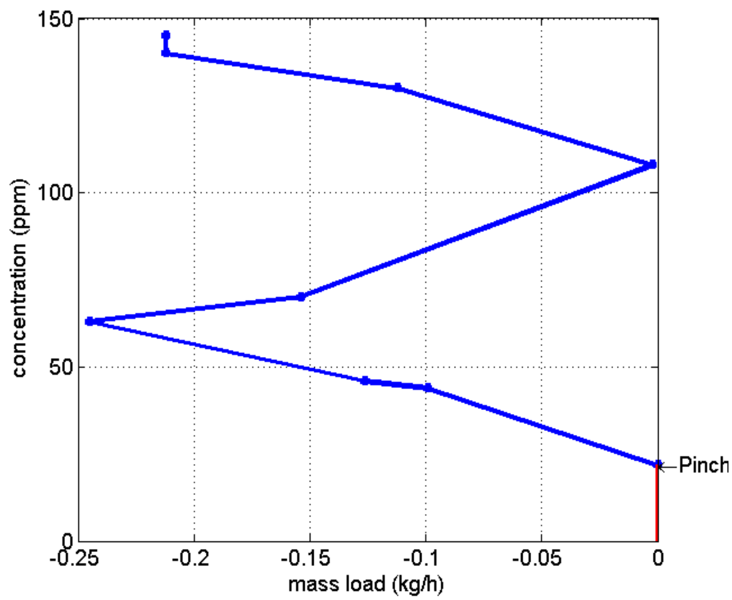

Figure 4.11.LCC and water supply line for Example 4.6

The pinch point locates on the lowest contaminant concentration (22 ppm). Column bottom is identified as a pinch-causing source, where the entire source is sent for the region below the pinch. The threshold concentration is also located on the highest concentration level. This means that all the process sinks are satisfied by process sources in terms of both flow rate and mass load requirement. Thus, this network does not require freshwater feed and yet generates no wastewater. The inverse slope of freshwater line (red line in Figure 4.11) identifies the zero freshwater flow rate target. As described earlier, the last segment of LCC, which is vertical for this example, shows the amount of total flow rate loss/gain. Zero wastewater flow rate is targeted because no total flow rate loss/gain exists.

Applying NNA, one possible water network is formed for Example 4.6 in Figure 4.12 as a matching matrix.

		F_{SKj} (ton/h)	6.5	8	12	4	10
		C_{SKj} (ppm)	46	63	63	130	140
F_{SRi} (ton/h)	C_{SRi} (ppm)	SK_j / SR_i	Stream	Second wash	Reactor	Hosepipes	First wash
4.5	22	Column bottom			4.45		0.05
9	44	Separator	6	2.15	0.85		
9	70	Second wash	0.5	5.85	2.65		
9	108	Reactor discharge			4.05		4.95
9	130	Dryer				4	5

Figure 4.12.Network design as matching matrix for Example 4.6

The same as in the two former examples, no forbidden matches region exist. Additionally, the mass balance equation for the lowest quality sink (First wash) does not hold.

4.6 Summary

CTA targeting method is initially developed for fixed flow problems. Unlike other FF targeting methods, CTA is more align with seminal work of WPA, i.e. Limiting Composite Curve method. The hybrid numerical and graphical characteristic of CTA provides not only conceptual insight to the problem but also numerical accuracy. It requires less calculation effort in contrast with other methodologies. For these reasons, this approach has been selected to handle diverse water network problems in reuse/recycle water scheme. The work of this chapter sets up the foundation for the following two chapters where regeneration water network will be addressed by extending CTA as a hybrid targeting method.

5. TOTAL WATER REGENERATION NETWORK OPTIMIZATION: FIXED POST REGENERATION CONCENTRATION

Considering regeneration-reuse/recycle scheme in water network synthesis opens more resource saving opportunities because water is treated partially in regeneration unit for further utilising within the network. Usually, for a total regeneration system, the freshwater and regenerated water flow rates are equal. However, in some cases, this consideration imposes infeasibility for the problem and freshwater flow rate should be lower (regeneration-recycling) or higher (partial regeneration) than regenerated water flow rate. Moreover, there are two classes of water regeneration units: the fixed post-regeneration (C_0) concentration type or the removal ratio (RR) type (Wang and Smith, 1994b).

As demonstrated in the previous chapter, CTA has the capability of handling diverse water network problems in reuse/recycle scheme. In this chapter, it is aimed to extend this targeting method for total regeneration water network for both fixed C_0 and RR type regenerator. The key parameters set before network design are freshwater, wastewater and regenerated water flow rates together with regeneration and wastewater concentrations. Note that, thus far, the other method which can address all of these key parameters for global water operations is the ultimate flow rate targeting (Ng et al., 2007b, 2008). Although this method is an excellent contribution, it lacks from several deficiencies:

- Iterative procedure is required for flow rate relocation between freshwater and regenerated water flow rate regions.
- Conceptual insight to the problem could not be provided due to its pure algebraic characteristic.
- It is limited to fixed C_0 problems.
- It is considered for only regeneration-recycle water network.

In view of the application limitation of previous studies, in this chapter, the CTA's numerical step is extended to set the targets for total regeneration water network with the assumption of specified C_0. Following problem statement, the procedure of so called Extended Composite Table Algorithm (ECTA) is described. The applicability is demonstrated by both FF and FL problems.

Nearest Neighbor Algorithm (NNA) is utilised to construct the network for FF problem, while Three Design Rules (TDR) is employed to form the process flow sheet for FL problem.

5.1 Problem statement

Figure 5.1 shows the superstructure presentation of the problem.

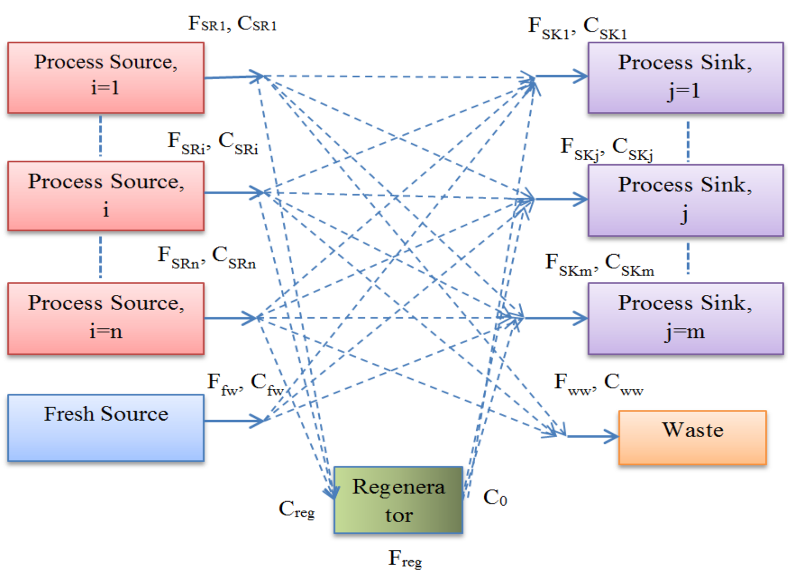

Figure 5.1.Source/sink presentation of regeneration water network

Consider a process that includes set of process sinks and set of process sources:

- Processes needing water are designated as Process Sinks or SK*j* (*j*=1, 2, … *m*). Each sink has a given flow rate, F_{SKj} and inlet concentration, C_{SKj}, which must satisfy: $C_{SKj}^{min} \leq C_{SKj} \leq C_{SKj}^{max}$, where C_{SKj}^{min} and C_{SKj}^{max}, is the lowest and the highest of concentration limit.

- Water-generating processes, which are reused or recycled to Process Sinks are designated as Process Source, or SRi (i= 1, 2,…, n), with a given flow rate of F_{SRi}, and an impurity concentration of C_{SRi}.
- Process sources are purified partially by given regeneration units with known performance index before recovering in the process sinks. As mentioned before, the performance of the regenerator can be assessed either by fixed post-regeneration (outlet regeneration) concentration (C_0) or by the removal ratio (RR) calculated by Eq. 5.1 (Wang and Smith, 1994b)

$$RR = \frac{C_{reg} - C_0}{C_{reg}} \tag{5.1}$$

C_{reg} is the inlet regeneration concentration. RR is defined as the ratio of the total mass load removal during the regeneration process to the amount of total impurity load entered to the regenerator by effluent stream. It is assumed that the flow rate loss for regeneration unit is negligible.

- When the process sources cannot fulfil the process sinks in terms of quality (contaminant mass load) and quantity (flow rate), an external freshwater source (regarded as a process source) with flow rate of F_{fw} and contaminant concentration of C_{fw} is introduced to satisfy the requirement of the process sinks. Unused water from process sources will be directed to the waste stream with the concentration of C_{ww} and flow rate of F_{ww}.

Given the above-described process, the flow rates of freshwater (F_{fw}), wastewater (F_{ww}), regenerated water (F_{reg}) along with the concentrations of regeneration (C_{reg}), post regeneration (C_0), and wastewater (C_{ww}) are the important parameters for a total water regeneration system. In this study, pure freshwater source (C_{fw} = 0 ppm) is supposed to serve the network. Since we are looking at the total water regeneration system, the flow rates of freshwater and regenerated water are considered to be identical.

The objective is to find minimum feasible F_{fw}, F_{reg}, F_{ww}, C_{reg}, and the corresponding C_{ww} with known C_0 and specified RR. Extended Composite Table

Algorithm (ECTA) is proposed in this chapter to target the key parameters in total regeneration network with the known C_0. In the following chapter (chapter 6), the assumption of fixed C_0 is relaxed through the newly developed targeting methodology, Composite Matrix Algorithm. Using the results achieved, the targets for RR type regenerator are set up. Then, based on the economic analysis of the total system, the optimum scenario which can meet the minimum total annual cost will be proposed.

5.2 Extended Composite Table Algorithm (ECTA)

Taking the concept proposed by Bai et. al. (2007), CTA is further developed to set the total water regeneration targets for global water operations. The first six steps of this method are the same as CTA (Agrawal and Shenoy, 2006) for targeting minimum freshwater flow (F_{fw}) rate and pinch concentration (C_{pr}) of reuse/recycle network. Detailed procedure can be found in Chapter 3. Two more steps are added for ECTA to target regenerated water flow rate (F_{reg}) and regeneration contaminant concentration (C_{reg}).

For the 7th step, interval regenerated water flow rates are calculated via Eq. 5.2 (Bai et al., 2007). The largest value among $F_{reg,k}$ targets the minimum regenerated water flow rate (F_{reg}) and the corresponding concentration is named freshwater pinch concentration (C_{pfw}). Based on the assumption of total regeneration network, the freshwater (F_{fw}) and regenerated (F_{reg}) water flow rates are identical. Note that the post regeneration concentration (C_0) is also a given value.

$$\begin{cases} F_{reg,k} = \dfrac{Cum.\Delta m_k}{2C_k - C_0} \\ \forall k \rightarrow C_0 \leq C_k \leq C_{pr} \end{cases} \tag{5.2}$$

For the 8th step, the interval regeneration concentrations are calculated by Eq. 5.3 (Bai et al., 2007). The minimum regeneration concentration (C_{reg}) is targeted by the maximum value among all $C_{reg,k}$. The associated concentration level is known as regeneration pinch concentration (C_{preg}).

$$\begin{cases} C_{reg,k} = \dfrac{Cum.\Delta m_k - F_{reg}(C_k - C_0)}{Freg} \\ \quad \forall k \to C_{pr} \le C_k \end{cases} \tag{5.3}$$

Wastewater flow rate (F_{ww}) and contaminant concentration (C_{ww}) targets are calculated by applying flow rate (Eq. 5.4) and mass balance (Eq. 5.5) over the total system, respectively. Note that the right side of Eq. 5.4 is the total flow rate loss/gain calculated through the ECTA procedure. The only unknown variable in Eq. 5.5 is the contaminant concentration of wastewater (C_{ww}).

$$F_{fw} - F_{ww} = \sum_j F_{SRj} - \sum_i F_{SKi} \tag{5.4}$$

$$F_{fw} \times C_{fw} - F_{ww} \times C_{ww} - F_{reg}(C_{reg} - C_0) = \sum_j F_{SRj} C_{SRj} - \sum_i F_{SKi} C_{SKi} \tag{5.5}$$

MATLAB is used as a programming tool to facilitate the implementation of ECTA. In the following, detailed application of ECTA is demonstrated via both FF and FL problems.

5.2.1 ECTA for FF water network problem

Example of Polley and Polley (2000) with the limiting data given in Table 5.1 is adopted.

Table 5.1.Limiting data for Example 5.1(Polley and Polley, 2000)

Sink	F_{SKj} (ton/h)	C_{SKj} (ppm)	Source	F_{SRi} (ton/h)	C_{SRi} (ppm)
SK1	50	20	SR1	50	50
SK2	100	50	SR2	100	100
SK3	80	100	SR3	70	150
SK4	70	200	SR4	60	250
Total	300		Total	280	

The main difference between CTA developed by Agrawal and Shenoy (2006) and ECTA proposed here is the last two columns of Table 5.2 for targeting regenerated water flow rate (F_{reg}) and regeneration contaminant concentration

(C_{reg}). The values in the 7th and 8th columns are calculated via Eqs. 5.2 and 5.3, respectively. Note the C_0 of 20 ppm is assumed for now.

Table 5.2.Implementation of ECTA for Example 5.1

1	2	3	4	5	6	7	8
k	C_k (ppm)	Net.F_k (ton/h)	Δm_k (kg/h)	Cum.Δm_k (kg/h)	$F_{fw,k}$ (ton/h)	$F_{reg,k}$ (ton/h)	$C_{reg,k}$ (ppm)
1	20			0	0	0	
2	50	50	1.5	1.5	30	18.75	
3	100	100	5	6.5	65	27.78	
4	**150**	80	4	10.5	**70**	**37.50**	150
5	200	10	0.5	11	55		113.33
6	**250**	80	4	15	60		**170**
7	(300)	20	(1)	(16)	(53.33)		(146.67)

The largest value of the 6th column is the required minimum pure freshwater flow rate target (70 ton/h) and its corresponding concentration level in column 2 is the pinch concentration (C_{pr} =150 ppm) for the reuse/recycle network. The minimum regenerated water flow rate (F_{reg}) is found as the largest value in the column 7 (37.5 ton/h) and its associated contaminant concentration (150 ppm) is the freshwater pinch concentration (C_{pfw}). Since the total water regeneration system is considered, the freshwater flow rate (F_{fw}) target is also 37.5 ton/h. The minimum regeneration concentration (C_{reg}) is set as 170 ppm with regeneration pinch concentration (C_{preg}) of 250 ppm. As it is observed from the last entry of Table 5.2, this system encounters total flow rate loss of 20 ton/h. Therefore, the wastewater flow rate (F_{ww}) is 17.5 ton/h and its contaminant concentration (C_{ww}) obtained via Eq. 5.5 equals 250 ppm. It is worth mentioning that Agrawal and Shenoy (2007) applied pure graphical method to achieve the same targeting results.

The LCC along with water supply lines created by MATLAB for this example is depicted in Figure 5.2.

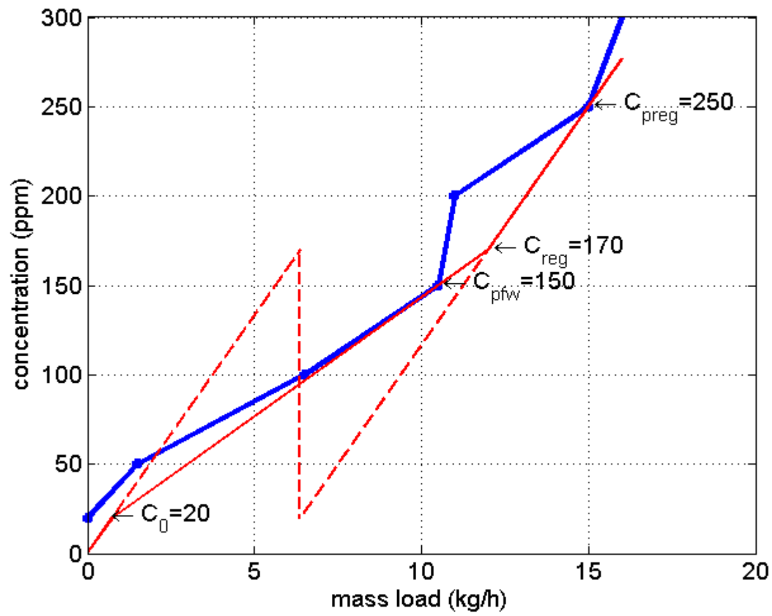

Figure 5.2.Limiting composite curve and water composite curve for total water regeneration network, where C_0 =20 ppm (Example 5.1)

As shown, the water composite curve (in red) is located entirely below the limiting composite curve (in blue) and intercepts the latter at two pinch points. This graphical presentation provides the conceptual insight for the problem and validates that the pre-specified targets obtained algebraically are feasible. One can refer to the previous works (Agrawal and Shenoy, 2006; Agrawal and Shenoy, 2007; Liao et al., 2007) to find the detailed procedure of constructing this graph.

Using of NNA network design method, one possible water network allocation is illustrated as a matching matrix in Figure 5.3. Notice that the outlet (Regout) and inlet (Regin) regeneration streams are considered as process source and sink, respectively. To design the network, the sinks are satisfied from the lowest to highest contaminant concentration.

		F_{SKj} (ton/h)	50	100	80	37.5	70	17.5
		C_{SKj} (ppm)	20	50	100	170	200	250
F_{SRi} (ton/h)	C_{SRi} (ppm)	SK_j / SR_i	SK1	SK2	SK3	Regin	SK4	WW
37.5	0	FW	7.5	27.5	2.5			
37.5	20	Regout	37.5					
50	50	SR1	5	45				
100	100	SR2		27.5	72.5			
70	150	SR3			5	30	35	
60	250	SR4				7.5	35	17.5

Figure 5.3.Network design for Example 5.1 as a matching matrix

The freshwater pinch concentration has been targeted as 150 ppm and the forbidden matches (across the pinch) are depicted as shaded cells in the matching matrix. This means that the available sources below the pinch concentration (including freshwater and regenerated water) cannot be utilised for the sinks in the lower quality region (above the pinch point). Similar to reuse/recycle water network, pinch causing source (SR3) is gain allocated to both regions. 5 ton/h of SR3 is allocated to higher quality region while the reaming flow rate (65 ton/h) is utilised in the lower quality region. Moreover, SR3 and SR4 are fed into regeneration unit to be purified and reused again for SK1. It is shown that, the identified targets can be achieved in practice through the network synthesis.

In comparison with pure reuse/recycle scheme, the inclusion of regeneration unit can possibly reduce up to 46% of the freshwater consumption and 65% of wastewater generation

5.2.2 ECTA for FL water network problem

The purpose of this section is to demonstrate the power of ECTA for targeting total water regeneration network (specifically total regeneration-reuse water network) considering FL operations. For this reason, the typical FL example (Wang and Smith, 1994b) is adopted. The limiting data and conversion to water sources and sinks are shown in Table 5.3. The same as in the literature, the post regeneration concentration (C_0) is assumed to be 5 ppm.

Table 5.3.Limiting Data for Example 5.2 (Wang and Smith, 1994b) and the conversion to FF model

		Limiting Data			
P_p	Δm_p (kg/h)	C_{in} (ppm)		C_{out} (ppm)	F_p (ton/h)
P1	2	0		100	20
P2	5	50		100	100
P3	30	50		800	40
P4	4	400		800	10
		Conversion to FF Model			
Sink	F_{SKj} (ton/h)	C_{SKj} (ppm)	Source	F_{SRi} (ton/h)	C_{SRi} (ppm)
$P1_{in}$	20	0	$P1_{out}$	20	100
$P2_{in}$	100	50	$P2_{out}$	100	100
$P3_{in}$	40	50	$P3_{out}$	40	800
$P4_{in}$	10	400	$P4_{out}$	10	800
Total	170		Total	170	

The procedure of ECTA is shown in Table 5.4. The regenerated (F_{reg}) and fresh (F_{fw}) water flow rate targets are 46.2 ton/h for total regeneration-reuse water network and the corresponding freshwater pinch concentration (C_{pfw}) is 100 ppm. The regeneration concentration (C_{reg}) and the regeneration pinch concentration (C_{preg}) are the same and equal to 100 ppm. Applying flow rate and mass load balances over the total system, wastewater flow rate (F_{ww}) and concentration (C_{ww}) are 46.2 ton/h and 793 ppm, respectively. This water system is a single pinch point network because all C_{pfw}, C_{reg}, and C_{preg} lie on each other. For verification, notice that the same targets were found through the Limiting Composite Curve Method (Wang and Smith, 1994b).

Table 5.4.Implementation of ECTA for FL problem (Example 5.2)

1	2	3	4	5	6	7	8
k	C_k (ppm)	Net.F_k (ton/h)	Δm_k (kg/h)	Cum.Δm_k (kg/h)	$F_{fw,k}$ (ton/h)	$F_{reg,k}$ (ton/h)	$C_{reg,k}$ (ppm)
1	0			0	0	0	
2	50	20	1	1	20	10.5	
3	<u>100</u>	160	8	9	<u>90</u>	<u>46.2</u>	<u>100</u>
4	400	40	12	21	52.5		60
5	800	50	20	41	51.3		93.3
6	(850)	0	(0)	(41)	(48.2)		(43.3)

To construct the total regeneration-reuse water network, TDR is a good candidate for such a FL problem. Some important points are necessary to explain for utilising TDR for this example. Therefore, the step by step network design is described as follows. TDR were described in Chapter 3 and recap here for convenience:

Rule 1: All units should have their maximum allowable outlet concentrations.

Rule 2: If the operations cross the pinch, the inlet concentration must be forced to the maximum allowable value. This rule can be easily carried out by NNA.

Rule 3: If the water-using processes are completely below or above the pinch, the cleanest available source is used to the maximum amount to satisfy these processes. Note that no sources from below the pinch should be used to satisfy the processes above the pinch and vice versa.

The process flow sheet is depicted in Figure 5.4. The network design is started from the most stringent process. P1 is a below-pinch unit which cannot tolerate any impurity. Thereof, pure freshwater (46.2 ton/h, 0 ppm) is used to satisfy this process. Considering Rule 1, the outlet concentration of P1 should be maintained to the maximum value. The required freshwater is calculated as 2000/(100-0)=20 ton/h, which is less than targeted amount (46. 2 ton/h). The outlet stream of P1 is 20 ton/h at 100 ppm.

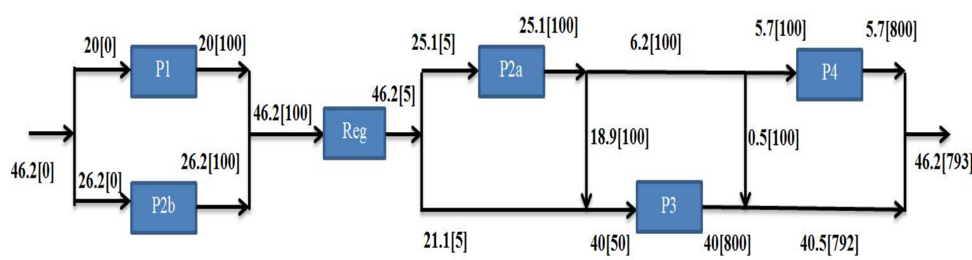

Figure 5.4.Process flow sheet for Example 5.2 (20[100] represents the stream with 20 t/h flow rate and 100 ppm concentration)

P2 is also a below-pinch unit. The available sources are fresh water (26.2 ton/h, 0 ppm), regenerated water (46.2 ton/h, 5ppm) and outlet stream of P1 (20 ton/h, 100 ppm). As per Rule 3, to satisfy this unit with cleanest available source (freshwater), 50 ton/h of this source is needed which is more than available freshwater amount (26.2 ton/h). Therefore, all of freshwater is exhausted and the next cleanest source (regenerated water) is utilised to pick up the remaining contaminant load. The corresponding flow rate is deduced as 2380/(100-5) =25.1 ton/h to keep the outlet concentration of P2 to the maximum amount. The outlet stream of P2 is 51.3 ton/h at 100 ppm.

P3 is an across-pinch operation with the maximum inlet concentration (50 ppm) below the pinch (100 ppm) and the maximum outlet concentration (800 ppm) above the pinch. Therefore, Rule 2 is applied for this unit to be satisfied. At this stage, the available sources are the remaining regenerated water (21.1 ton/h, 5ppm), the outlet stream of P1 (20 ton/h, 100ppm), and the outlet stream of P2 (51.3 ton/h, 100 ppm). For the inlet of P3 (50 ppm), the just cleaner neighbor source is regenerated water and the just dirtier one is the outlet of either P1or P2. However, careful inspection of available water sources reveals that the P2 needs both fresh water (26.2 ton/h) and regenerated water (25.1 ton/h) to be fulfilled. Consequently, it is essential to decompose this process to below (P2b) and above regeneration (P2a) process to have a total regeneration-reuse water network. The same practice also was done in the literature (Bai et al., 2010; Mann and Liu, 1999; Wang and Smith, 1994b). Considering this issue, the outlet stream of P2a (25.1 ton/h, 100 ppm) and the remaining regenerated water flow rate are chosen as the nearest neighbor to meet the P3 mass load requirement. Using the two equations for NNA (Eqs. 3.5 & 3.5), gives the 21.1 ton/h of regenerated water along with 18.9 ton/h of P2a outlet stream to satisfy the P3. Knowing the fact that the regeneration unit is located across the P2b and P2a unit and the regenerated water flow rate (F_{reg}) and inlet regeneration concentration (C_{reg}) are 46.2 ton/h and 100 ppm, respectively, the outlet of P1 (20 ton/h, 100 ppm) and the outlet of P2b (26.2, 100 ppm) are considered as the sources to be fed to the regeneration unit (46.2 ton/h, 100 ppm).

P4 is an above-pinch operation. Rule 3 is considered and also the outlet concentration of the unit (800 ppm) should be maintained. At this stage, the available sources are 40 ton/h of P3 outlet stream at 800 ppm and outlet stream of

P2a (6.2 ton/h, 100 ppm). Hence, 5.7 ton/h (4000/(800-100)) of the cleanest available source above the pinch (P2a outlet stream) is reused to P4. By this stage, not only all the processes are satisfied, but also all the targets obtained via ECTA are achieved through network design.

It is also worthy to mention that, as long as the targets can be determined accurately in WPA studies, one can employ any other network design tool such as water grid diagram (Mann and Liu, 1999; Wang and Smith, 1994b) or mass content table (Mann and Liu, 1999) to design the network in FL model. This is also applicable for FF operations; however, the only design tool reported for water regeneration network is NNA (Agrawal and Shenoy, 2006; Deng and Feng, 2011).

Recently, Shenoy (2012) developed unified water network design method for both FF and FL problems. However, the applicability of this method was just demonstrated for reuse/recycle water network and zero water discharge with inclusion of regeneration unit. The extension of this method to total water regeneration network can be considered as a future research direction

5.3 Summary

In this chapter, Extended Composite Table Algorithm (ECTA) has been proposed to target all the key parameters of total water regeneration network. The contributions of this study are highlighted as below.

- Agrawal and Shenoy (2006) used CTA to construct the LCC. Then, on the basis of this graphical presentation the targets for total water regeneration network were determined. Therefore, although, all the key parameters of total water regeneration can be set through this approach for global water operations, it is not completely reliable for highly integrated water network. The interpretation of the graphical presentation can be very tedious when the turning points of LCC are not clearly distinguishable. Moreover, this approach may fail for the special multiple pinch case (similar to Example 5.1) (Agrawal and Shenoy, 2007; Bai et al., 2007; Liao et al., 2007).

- The extended Mass Problem Table proposed by Bai et al. (2007) to set the targets algebraically for total water regeneration network is limited to FL operations. The ECTA proposed in this study can handle global water operation (FL and FF) for more generic problems (without the restriction of limiting composite curve shape) in a hybrid manner (both algebraically and graphically).

However, ECTA is developed based on the assumption of total water regeneration network (F_{fw}=F_{reg}). In some cases regenerated water flow rate should be either lower or higher than freshwater flow rate in order to meet the feasibility of the problem (Feng et al., 2007) and this will be the scope of future studies.

6. TOTAL WATER REGENERATION NETWORK OPTIMIZATION: RELAXED POST REGENERATION CONCENTRATION

The performance of water regeneration unit is judged by two criteria (1) specified post-regeneration concentration (C_0); (2) specified removal ratio (RR). Most of pinch analysis methods have considered the first criterion for targeting regeneration-reuse/recycle network (Agrawal and Shenoy, 2006; Bai et al., 2007; Castro et al., 1999; El-Halwagi, 2006; Foo et al., 2006; Hallale, 2002; Kuo and Smith, 1998a; Manan et al., 2004; Mann and Liu, 1999; Ng et al., 2007b). A little attention has been paid to the second one (Bandyopadhyay and Cormos, 2008; Wang and Smith, 1994b). Wang and Smith (1994b) addressed water network synthesis inclusion of RR type regenerator. Nevertheless, they dealt with very simple single pinch problem and it is restricted to fixed load water operations. Although, Source Composite Curve (Bandyopadhyay and Cormos, 2008) can handle RR type regenerator, it only locates the target for regeneration-recycle network and very special case of zero liquid discharge.

The performance of water regeneration unit has the dominant influence on the total cost of network because decreasing C_0 (increasing RR) leads to the increase of the capital and operating costs of regenerator exponentially (Feng and Chu, 2004).

Due to the afore-mentioned facts, in this chapter, ECTA (Chapter 5) is further improved by including a procedure for finding feasible region corresponding to a relaxed post regeneration concentration. The problem statement was given in the previous chapter. The so called Composite Matrix Algorithm (CMA) can find targets for a network with any specified RR type regenerator and be useful for the study of total water regeneration network on economic basis.

6.1 Composite Matrix Algorithm (CMA)

CMA is developed to define the feasible range of key variables for total water regeneration network. In this method, post-regeneration concentration (C_0)

increases from the minimum (C_0^{min}) to maximum (C_0^{max}) with an incremental step of Δ. In each step, for a given C_0, regenerated flow rate is calculated at every concentration level. The maximum value is extracted to generate a feasible vector of minimum regenerated and freshwater flow rates across the entire C_0 range [C_0^{min}, C_0^{max}]. The same operation will generate a matrix of regeneration concentration and the vector of feasible regeneration concentration is extracted by choosing the maximum value in every column of this matrix. In addition, the vectors of freshwater and regeneration pinch concentration, wastewater flow rate, and wastewater concentration can also be derived. Following this method, it is possible to construct the feasible region along with the Limiting Composite Curve (LCC) and target the system for specified RR regeneration type. The trade-off between the parameters can be studied quantitatively and it will give a chance to analyse the network economically.

The example of Polley and Polley (2000) with the limiting data provided in the previous chapter (Example 5.1) is revisited to describe the procedure of CMA explicitly. One important concept is essential to be discussed before describing the procedure of CMA. By increasing the C_0, the minimum freshwater flow rate (F_{fw}) in total regeneration system increases. In the LCC, F_{fw} is calculated by the inverse slope of the first segment of water supply composite curve below the C_0. Therefore, increasing the C_0 causes the freshwater flow rate segment approaching the LCC and finally intersects it in C_0^{max} (Figure 6.1). For any C_0 higher than C_0^{max}, water supply composite curve will cross the LCC and this imposes infeasibility on the problem. Therefore, identifying C_0^{max} is crucial for the determination of feasible region of parameters under study in the total regeneration system. Without loss of generality, C_0^{max} can be located at either the reuse/recycle pinch point (C_{pr}) or any point on the LCC lower than C_{pr} depending on the shape of LCC. Figure 6.1 shows three water supply composite curves for C_0s of 10, 35, and 65 located below the LCC for illustrating the concept.

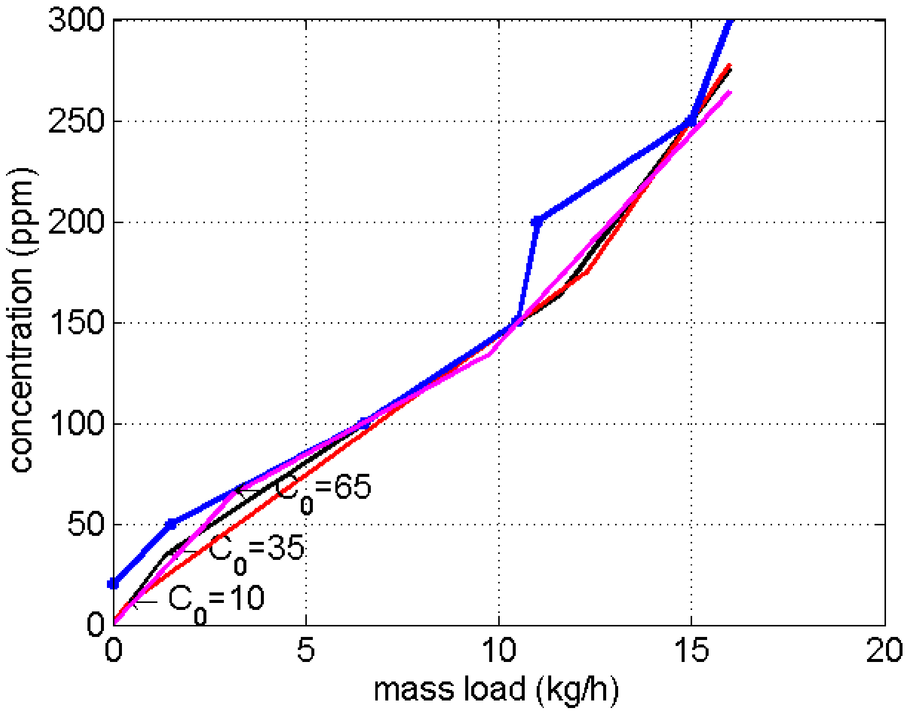

Figure 6.1.LCC along with water supply composite curves for C_0s chosen as 10, 35, and 65

The procedure of CMA is summarized in Figure 6.2 to provide a clear depiction of the proposed algorithm.

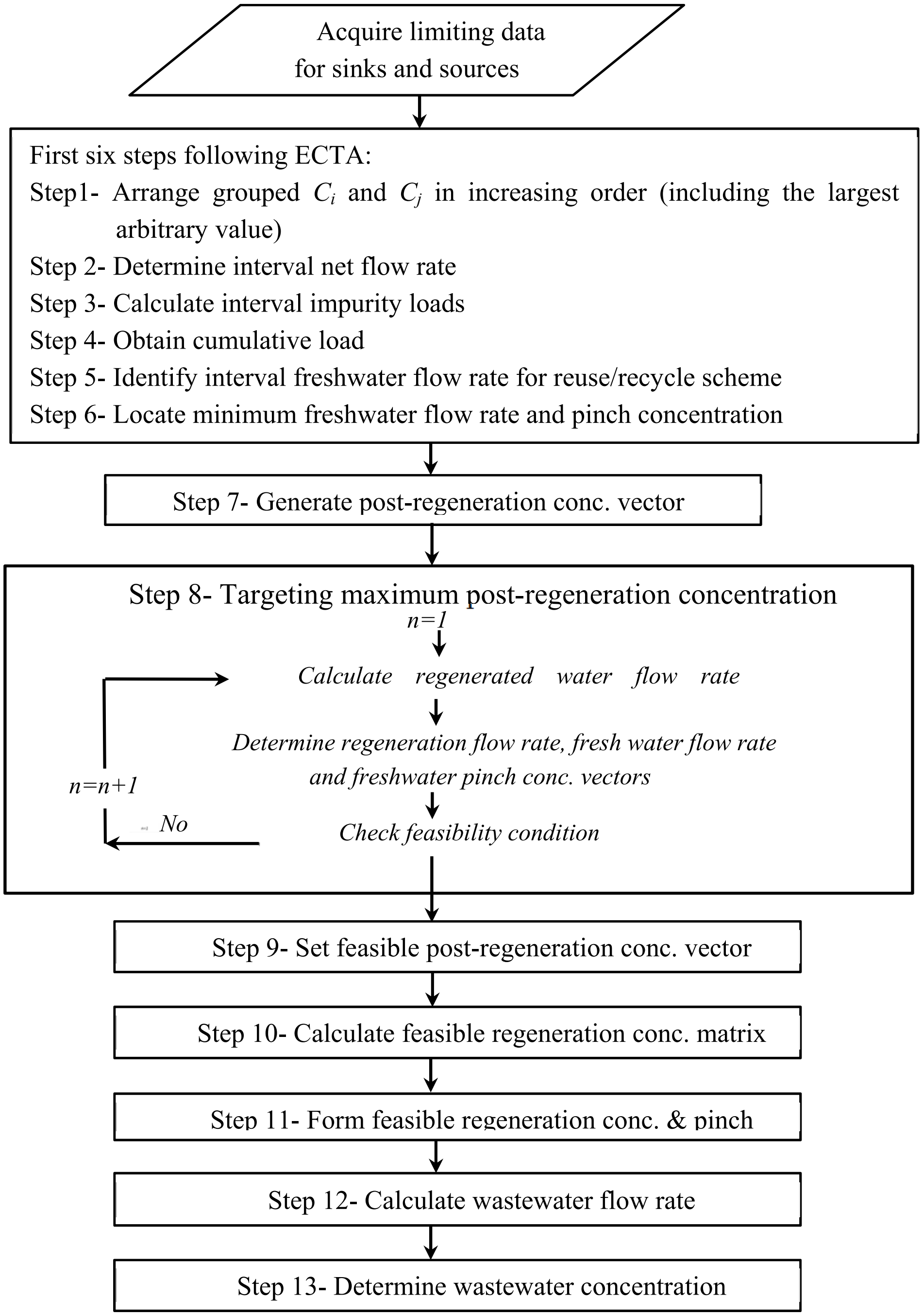

Figure 6.2.Flowchart for Composite Matrix Algorithm

Step 1-6. Targeting minimum freshwater flow rate and pinch point concentration

The first six steps of CMA are the same as ECTA (Chapter 5). From those steps, the pinch point concentration (C_{pr}) and minimum freshwater flow rate (F_{fw}) for reuse/recycle network can be determined.

Step 7. Generate the post-regeneration concentration vector

This step of CMA method produces the vector of post regeneration concentrations via Eq. 6.1. Incremental step (Δ), and C_0^{min} have been set to be 0.1 and 1, respectively. As discussed, C_0^{max} cannot be higher than reuse/recycle pinch concentration (C_{pr}). Therefore, C_0^{max} is considered as 150 ppm (set via ECTA) and this will be updated later through the CMA method if necessary. Applying these constraints, Eq.6.1 generates the vector of $\mathbf{C_0}$= [1, 1.1, 1.2,…, 150]^T where $n \in N'$ =1, 2, 3, …..,1491

$$\begin{cases} C_{0,n} = C_0^{\min} + \Delta \\ C_0^{\min} \le C_{0,n} \le C_0^{\max} \\ \forall n \in N' = 1,2,\ldots,\dfrac{C_0^{\max} - C_0^{\min}}{\Delta} + 1 \end{cases} \tag{6.1}$$

Step 8. Targeting maximum post-regeneration concentration

Step 8 is a close loop iteration process and consists of several sub-steps as follows:

(a) Identify regenerated water flow rate matrix

In this sub-step, regenerated water flow rate ($MF_{reg,kn}$) is calculated via Eq. 6.2 for each $C_{0,n}$. Concentration level (C_k) between post-regeneration concentration ($C_{0,n}$) and reuse/recycle pinch concentration (C_{pr}) should be taken into account for each iteration. Hence, this equation is the extension of Eq. 5.2 allowing the post-regeneration concentration to increase between the minimum and maximum values. In the other words, every column of regenerated water flow rate matrix consists of the values located in the 7th column of Table 5.2 for a specified post-regeneration concentration.

$$\begin{cases} MF_{reg,kn} = \dfrac{Cum.\Delta m_k}{2C_k - C_{0,n}}; \\ \forall n, k \rightarrow C_{0,n} \le C_k \le C_{pr} \; \& \; \forall n \in N' \end{cases} \qquad (6.2)$$

(b) Determine regeneration flow rate, freshwater flow rate and freshwater pinch concentration vectors

The maximum value in every column of $\boldsymbol{MF}_{\mathbf{reg}}$ is extracted and stored in the regeneration flow rate vector ($\boldsymbol{F}_{\mathbf{reg}}$). Based on the assumption of total regeneration scheme, every value in $\boldsymbol{F}_{\mathbf{reg}}$ is equal to freshwater flow rate, i.e. $\boldsymbol{F}_{\mathbf{fw}} = \boldsymbol{F}_{\mathbf{reg}}$. The corresponding concentration level (C_k) to every value in $\boldsymbol{F}_{\mathbf{fw}}$ is set as freshwater pinch concentration.

(c) Check the feasibility condition of post-regeneration concentration

As discussed earlier, with the increase of post-regeneration concentration (C_0), the freshwater segment of water supply composite curve gets closer to LCC and finally touches it. In this sub-step, the feasibility condition of increasing C_0 is necessarily checked.

Constructing the freshwater line formula: Freshwater line is the first segment of water supply composite curve located below the C_0 (refer to Figure 6.3). Defining line AB as the fresh water supply line, for every iteration, the points of A and B can be determined using Eq. 6.3. Note that according to the assumption of pure fresh water availability, C_{fw} is set to zero. Furthermore, cumulative mass load (Cum.Δm_k) corresponding to the first concentration level is also zero (Table 5.2). Hence, x-y coordinates of point A are zeroes for all iterations.

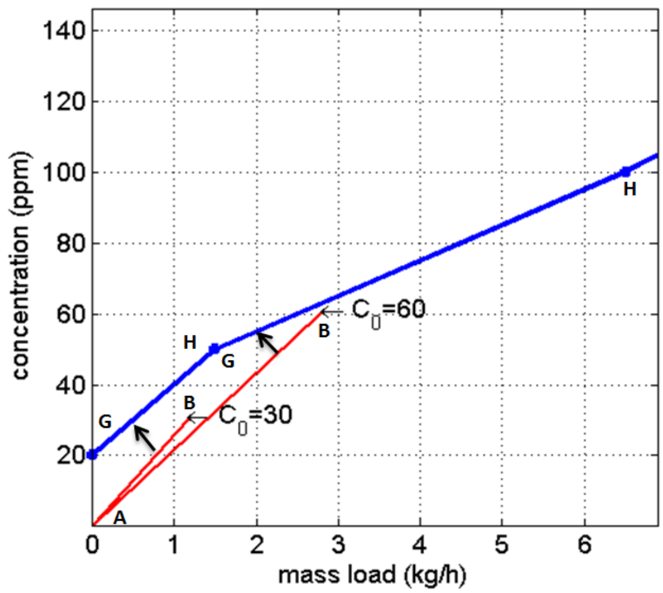

Figure 6.3.Freshwater lines and LCC segments for C0s of 30 and 60

$$A = \left| \begin{matrix} Cum.\Delta m_k & \quad \forall k = 1 \\ C_{fw} & \end{matrix} \right. \qquad B_n = \left| \begin{matrix} (C_{0,n} - C_{fw}) \times F_{reg,n} \\ C_{0,n} \end{matrix} \right. \quad \forall n \in N' \quad (6.3)$$

Determining limiting composite curve segment formula: Points G and H (Eq. 6.4) are the two following LCC points. The y-coordinate of point H must be equal or higher than the y-coordinate of point B of freshwater line. Therefore, GH line (Figure 6.3) equation identified in every iteration represents the LCC segment approached by the freshwater line.

$$\begin{cases} G_n = \left| \begin{matrix} Cum.\Delta m_{k-1} \\ C_{k-1} \end{matrix} \right. \qquad H_n = \left| \begin{matrix} Cum.\Delta m_k \\ C_k \end{matrix} \right. \\ \forall n, k \rightarrow C_{0,n} \leq C_k \ \& \ \forall n \in N' \ \& \ \forall k \geq 2 \end{cases} \qquad (6.4)$$

Freshwater lines and LCC segments for C_0s of 30 and 60 are shown in Fig. 6.3 for the purpose of clarification.

The intersection of AB and GH lines is thus found and the corresponding y-coordinate is stored in **y_intersect** vector. The feasibility condition is checked via Eq. 6.5.

$$\begin{cases} 0 < y\_intersect_n - C_{0,n} \leq \varepsilon \\ \qquad \forall n \in N' \end{cases} \tag{6.5}$$

ε for this example is set to be 0.05. This condition ensures that the maximum feasible freshwater line (which its inverse slope targets the maximum feasible freshwater flow rate) associated with the maximum post regeneration concentration (C_0^{max}) is located below and very close to LCC. Hence, for every iteration, the condition should be checked. If it does not meet the accuracy requirement, the procedure goes back to step (a). Otherwise, $C_{0,n}$ is set to be the C_0^{max} and the procedure is moved to the next step.

Although, decreasing Δ and ε simultaneously leads to achieving more accurate C_0^{max}, this causes longer computational time. In fact, our study on varying these two parameters showed the current values are reasonable and further decrease does not affect the final results (i.e. targeting for RR type regeneration unit and cost evaluation).

As a result of the above procedure, the feasible freshwater flow rate ($\boldsymbol{F}_{\mathbf{fw}}$), regeneration flow rate ($\boldsymbol{F}_{\mathbf{reg}}$), and freshwater pinch concentration ($\boldsymbol{C}_{\mathbf{pfw}}$) vectors are formed and the maximum feasible post-regeneration concentration (C_0^{max}) is set up. For the purpose of clarity, the quantified regenerated water flow rate matrix and vector, and freshwater pinch concentration vector for three random iterations with C_0s of 10 ppm, 40 ppm and 65 are shown below:

$$\begin{array}{c c} & \begin{array}{ccccccccc} \ldots & 10 & \ldots & 40 & \ldots & 65 & \ldots \end{array} \\ F_{reg,4\times690} = \begin{array}{c} 20 \\ 50 \\ 100 \\ 150 \end{array} & \begin{bmatrix} \ldots & 0 & \ldots & 0 & \ldots & 0 & \ldots \\ \ldots & 16.67 & \ldots & 25 & \ldots & 0 & \ldots \\ \ldots & 34.21 & \ldots & 40.62 & \ldots & 48.15 & \ldots \\ \ldots & 36.21 & \ldots & 40.38 & \ldots & 44.68 & \ldots \end{bmatrix} \Rightarrow F_{fw,690} = F_{reg,690} = [\ldots 36.21 \ldots 40.62 \ldots 48.15 \ldots]^T \end{array}$$

$$\Rightarrow C_{pfw,690} = [\ldots\ldots 150 \ldots\ldots 100 \ldots\ldots 100 \ldots\ldots]^T$$

The values located on the left and top outside of the matrix are just the indication of concentration levels (lower than reuse/recycle pinch concentration) and post-regeneration concentrations, respectively. freshwater pinch concentration vector ($\boldsymbol{C}_{\mathbf{pfw}}$) contains freshwater pinch concentrations for every post-regeneration concentration (C_0). This quantified vector depicts that with the increase of C_0, the freshwater pinch point switches from one turning point of LCC to another point located lower than the original one. This fact is controlled by the shape of LCC and it is totally dependent on the limiting data of process sources and sinks. The C_0 which causes this phenomenon is given the name of "transient post regeneration concentration (C_{0tr})" in this research and will be investigated further later.

Additionally, the maximum post-regeneration concentration (C_0^{max}) for this example is targeted to be 69.9 ppm.

Step 9. Set feasible post-regeneration concentration vector

The post-regeneration concentration vector ($\boldsymbol{C_0}$) is updated using the targeted C_0^{max} (for this example 69.9 ppm) in Eq. 6.1. The new range of $\boldsymbol{C_{0,n}}$ is produced where $\forall n \in N$ =1,2,……, 690.

Step 10. The calculation of feasible regeneration concentration matrix

In this step, the feasible regeneration concentration $MC_{reg,kn}$ is calculated via Eq. 6.6 which is the extended of Eq. 5.3. With all the parameters known, feasible regeneration concentration matrix is formed by considering all concentration levels, which are equal or greater than reuse/recycle pinch concentration and all feasible post-regeneration concentrations. Specifically, every column of $\mathbf{MC_{reg}}$ comprises the values located in the 8th column of Table 5.2 for a specified C_0.

$$\begin{cases} MC_{reg,kn} = \dfrac{Cum.\Delta m_k - F_{reg,n}(C_k - C_{0,n})}{Freg_n} \\ \forall k,n \rightarrow C_{pr} \le C_k \;\&\; \forall n \in N \end{cases}; \qquad (6.6)$$

Step 11. The extraction of feasible regeneration concentration vector and regeneration pinch concentration vector

The maximum value in every column of $\mathbf{MC_{reg}}$ determines the minimum regeneration concentration associated to every feasible post regeneration concentration. Therefore, extracting these values forms the regeneration concentration vector ($\boldsymbol{C}_{\mathbf{reg}}$). In addition, the corresponding concentration levels to all of these values are stored in the regeneration concentration pinch vector ($\boldsymbol{C}_{\mathbf{preg}}$).

The schematic $\mathbf{M}\boldsymbol{C}_{\mathbf{reg}}$, $\boldsymbol{C}_{\mathbf{reg}}$, and $\boldsymbol{C}_{\mathbf{preg}}$ for C_0s of 10 ppm, 40 ppm, and 65 ppm are as follows:

$$
MC_{reg,4\times 690} = \begin{array}{c} \\ 150 \\ 200 \\ 250 \\ 300 \end{array}
\begin{array}{c} \begin{array}{ccccccccc} \ldots & 10 & \ldots & 40 & \ldots & 65 & \ldots \end{array} \\
\begin{bmatrix} \ldots & 150 & \ldots & 148.46 & \ldots & 133.08 & \ldots \\ \ldots & 113.81 & \ldots & 110.77 & \ldots & 93.46 & \ldots \\ \ldots & 174.29 & \ldots & 159.23 & \ldots & 126.54 & \ldots \\ \ldots & 151.90 & \ldots & 113.85 & \ldots & 97.31 & \ldots \end{bmatrix} \end{array}
\Rightarrow C_{reg,690} = [\ldots174.29\ldots\ldots159.23\ldots\ldots133.08\ldots]^T
$$

$$
\Rightarrow C_{preg,690} = [\ldots\ldots250\ldots\ldots250\ldots\ldots150\ldots]^T
$$

The considered concentration levels and post-regeneration concentrations are indicated left and top outside of the regeneration concentration matrix, respectively for better illustration. As seen from $\boldsymbol{C}_{\mathbf{preg}}$, the regeneration pinch concentration switches from 250 ppm to 150 ppm at transient post regeneration concentration which will be targeted later in this study.

Step 12. Calculate wastewater flow rate vector

The wastewater flow rate ($F_{ww,n}$) can be readily calculated via Eq. 6.7. The total flow rate loss/gain (20 ton/h flow rate loss) is independent of C_0. Therefore, all the wastewater flow rates associated to different C_0s are 20 ton/h less than the freshwater flow rates.

$$
\begin{cases} F_{fw,n} - F_{ww,n} = \sum_j F_{SKj} - \sum_i F_{SRi} \\ \forall n \in N \end{cases} \qquad (6.7)
$$

Step 13. Determine the wastewater concentration vector

Eq. 6.8 is a modified version of Eq. 5.5 to calculate the wastewater concentration vector ($\boldsymbol{C}_{\mathbf{ww}}$). For C_0s of 10 ppm, 40 ppm, 65 ppm, the wastewater concentrations are identified as 250 ppm, 250 ppm, 238.82 ppm.

$$\begin{cases} -F_{ww,n} \times C_{ww,n} - F_{reg,n} \times (C_{reg,n} - C_{0,n}) = \sum_j F_{SKj} C_{SKj} - \sum_i F_{SRi} C_{SRi} \\ \forall n \in N \end{cases} \tag{6.8}$$

6.2 Using the CMA results

The CMA results give the opportunity to set the feasible region for the problem, to target the water network for RR type regenerator, and to evaluate the total system on the economic basis. These issues are discussed in the following sections.

6.2.1 Feasible region for total water regeneration network

Since, for every post regeneration concentration, CMA gives the regenerated water flow rate and the regeneration concentration, it is possible to construct water supply composite curves for each set of these values. In Figure 6.4, water supply composite curves are drawn based on the feasible post-regeneration concentration vector (**C_0**), regenerated water flow rate vector (**$F_{reg} = F_{fw}$**), and regeneration concentration vector (**C_{reg}**). These curves form a feasible region for the problem under consideration.

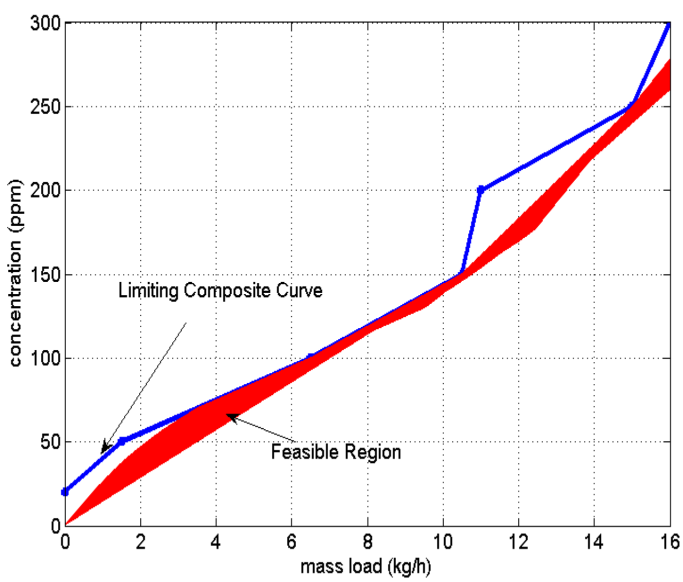

Figure 6.4.Limiting composite curve along with feasible region for total water regeneration network

It can be seen that the feasible region for total water regeneration network is located entirely below the LCC. This meets the constraints for water network synthesis. Further studies for targeting the network with specified RR regenerator and finding the optimum total cost scenario are all conducted within these constraints so that the results are guaranteed to be feasible.

6.2.2 Targeting from Removal Ratio (RR) graph

The definition of RR (Eq. 5.1) is firstly modified to accommodate vector calculation (Eq. 6.9). Since CMA sets the feasible range of regeneration and post-regeneration concentrations at the first instant, Eq. 6.9 produces the feasible range of RR as well.

$$\begin{cases} RR_n = \dfrac{C_{reg,n} - C_{0,n}}{C_{reg,n}}; \\ \qquad \forall n \in N \end{cases} \tag{6.9}$$

Plotting $C_{0,n}$, $C_{\mathrm{reg},n}$, $C_{\mathrm{ww},n}$, $C_{\mathrm{pfw},n}$, $C_{\mathrm{preg},n}$, $F_{\mathrm{reg},n}$, $F_{\mathrm{fw},n}$, and $F_{\mathrm{ww},n}$ versus RR_n for every $n \in N$ gives an overall picture of targeted water network with the regenerator specified by RR (Figure 6.5). For any specified removal ratio, the contaminant concentration targets can be found in Figure 6.5a and relevant flow rate targets can be identified from Figure 6.5b.

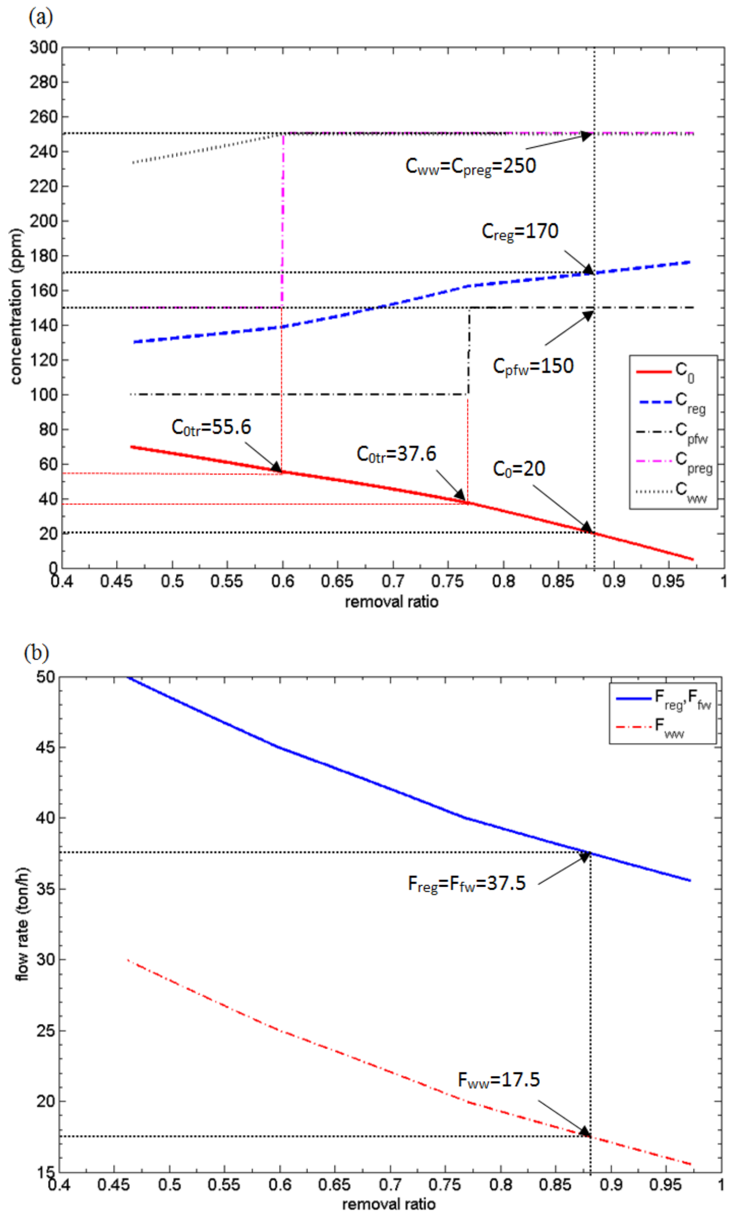

Figure 6.5.Removal Ratio graph shows the relationship between Removal Ratio and (a) concentrations (b) flow rates.

To use this graph, for instance, the regeneration unit with 88% RR performance index is assumed, drawing a vertical line from the given RR index intersects any of the graphs presented. The projection of these intersections on the y-axis identifies the targets for total water regeneration network. C_0, C_{reg}, F_{reg} and F_{ww} are targeted as 20 ppm, 170 ppm, 37.5 ton/h, and 17.5, respectively. For this specified performance index, the freshwater pinch concentration (C_{pfw}) and regeneration pinch concentration (C_{preg}) are found to be 150 ppm, and 250 ppm, respectively. The same targets were reported for a specified C_0 of 20 ppm in the literature (Agrawal and Shenoy, 2007; Liao et al., 2007) and are set via ECTA in Chapter 5. Moreover, one possible network design for the total water regeneration system considering these targets is demonstrated in the previous chapter (Figure 5.3).

Therefore, using the results from CMA, it is possible to establish removal ratio graph for a water network problem. With any specified RR type regenerator included, the targets can be easily obtained.

6.2.3 The pinch point migration and minimum feasible RR

As illustrated in Figure 6.5a, freshwater pinch concentration (C_{pfw}) switches from 150 ppm to 100 ppm at the post-regeneration concentration of 37.6 ppm. The same phenomenon also happens for regeneration pinch concentration (C_{preg}) at the C_0 of 55.6 ppm, where, the pinch point migrates from 250 ppm to 150 ppm. It is noticed that the concave turning points of LCC are controlling this kind of pinch movement. As an example, there is another concentration level (200 ppm) between 150 and 250 ppm (Table 5.2), but, it is impossible for 200 ppm to be considered as a potential pinch point. Moreover, depending on the distinct shape of limiting composite, the pinch migration may not happen, or, on the other hand, may occur several times. For this particular example, two transient post regeneration concentrations (C_{0tr}) which cause pinch movement are found as 37.6 ppm and 55.6 ppm. Further to these observations, pinch points are always migrated (if applicable) from higher to lower concentration level with the increase of C_0 in total water regeneration system.

The other specific feature of the RR graphs is the minimum feasible performance of the regeneration unit. In this example, the regeneration unit with the performance lower than 46% cannot serve this water network due to the occurrence of mass load infeasibility. An uncovered lower part of removal ratio (Figure 6.5) gives this conceptual insight.

6.3 Economic evaluation of total system

The higher quality regenerated water (lower C_0, or higher RR) leads to the less demand for freshwater supply and consequently less waste disposal. This is because the higher quality in-plant purified water (regenerated water) would permit more water reuse/recycle after regeneration unit. On the other hand, the total cost of treatment unit increases dramatically with higher regenerator performance. It can be concluded that one of the most important factors in the optimization of water regeneration–reuse/recycle network is the performance of regeneration unit, which is determined by C_0 or RR. However, not much attention has been given to the influence of these parameters to the total network cost (Feng and Chu, 2004). Post-regeneration concentration (C_0) has been assumed to be fixed for most of the pinch analysis targeting methods. Our CMA method relaxes the post regeneration concentration, therefore, provides an opportunity to study the network from more practical point of view.

6.3.1 Cost functions

One can analyse the interaction between the parameters through CMA method for total water regeneration network. This will further give a chance to optimize the network on economic basis by setting a cost function.

The cost of freshwater supply (CF), disposal treatment (CD), and regeneration process (CR) are taken into account in this work. As stated, the lower C_0 (higher RR) results in the lower freshwater requirement. This also can be clearly observed in Figure 6.5b. Therefore, the freshwater supply cost (CF) also decreases with the decrease of C_0. Using the same case as an example, it is supposed that the water system is working 8600 h/yr and the freshwater supply cost is considered to be 1$/ton. Please note that all the cost functions and coefficients are given based on the US dollar.

The governing parameters for regeneration unit are: regeneration flow rate (F_{reg}), post-regeneration concentration (C_0), and contaminant regeneration load (M_{reg}) which is expressed by Eq. 6.10.

$$M_{reg} = F_{reg} \times (C_{reg} - C_0) \qquad (6.10)$$

Substituting the regeneration flow rate, regeneration concentration and post-regeneration concentration vectors obtained from CMA in Eq. 6.10, the feasible range of contaminant regeneration load is determined. Figure 6.6 illustrates the interaction between C_0, F_{reg} and, M_{reg}.

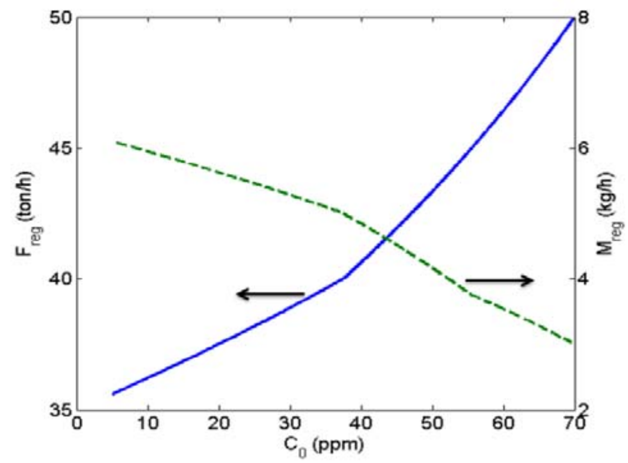

Figure 6.6.Trade-off between C_0, M_{reg}, F_{reg}

With the increase of C_0, although the regenerated water flow rate increases, the mass load picked by regenerator reduces. This means that the function of regeneration unit in total system gradually diminishes and the water network moves towards the pure reuse/recycle configuration. Therefore, if the saving of the resources is the main objective, higher performance of the regeneration unit (lower C_0) is a better choice. However, the total cost of regeneration (including operating and capital costs) rises exponentially in order to produce higher quality water (Feng and Chu, 2004). Hence, selecting high performance regenerator (assumed in most of WPA studies) may not guarantee the optimum total cost of the network.

The expression for total regeneration cost is adopted from Feng and Chu (2004) and modified here as Eq. 6.11. It includes annualized capital cost and operating cost and is a function of regeneration flow rate and post-regeneration concentration.

$$\begin{cases} CR_n = \alpha \times F_{reg,n}{}^{\beta} \times \left(\dfrac{C_0{}^{\max}}{C_{0,n}} \right)^{\gamma} \\ \forall n \in N \end{cases} \tag{6.11}$$

Note that $C_0^{\max}$ is a constant value which can be found through the CMA method in the preceding sections. β and γ are taken from the literature (Feng and Chu, 2004) to be 0.14 and 1.75, respectively. With 8600 h/yr of operating cost, α is set for 15 and CR gives the cost in k$/yr. From Eq. 6.11, it can be clearly noticed that the C_0 and F_{reg} are competing with each other in terms of cost. Therefore, this cost function is in agreement with our discussion about the trade-off between key parameters in the regeneration unit.

For the calculation of wastewater disposal charge, it is essential to consider both quantity (F_{ww}) and quality (C_{ww}) of wastewater. The feasible range for these parameters has been identified before and the correlation between C_0, F_{ww}, and C_{ww} is depicted in Figure 6.7.

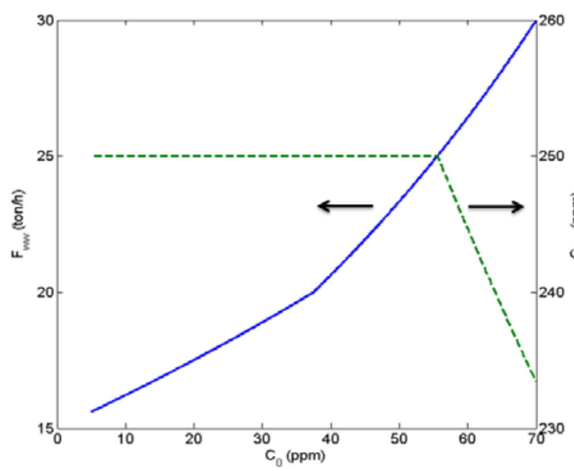

Figure 6.7.Interaction between C_0, F_{ww}, and C_{ww}

The trend of wastewater produced with the increase of C_0 is identical to that of freshwater intake with 20 ton/h lag due to water loss in the network. However, the change of effluent contaminant concentration (C_{ww}) to the increase of C_0 does not follow one specific pattern for the whole range of C_0 in this example as shown in Figure 6.7. It is a plateau (250 ppm) for some extent then it declines gradually. Although, there is not one particular trend here, the concentration of wastewater cannot be increasing with the rise of C_0 for any cases. The lower quality of regenerated water gives less chance for reuse/recycle after regeneration unit. This fact may cause the reduction of C_{ww}.

The Mogden Formula (Kim, 2012) is rearranged and modified as Eq. 6.12 to consider the operating cost of wastewater treatment.

$$\begin{cases} CD_n = (A + (B \times \frac{C_{ww,n}}{Ss})) \times F_{ww,n} \\ \forall n \in N \end{cases} \qquad (6.12)$$

Where: A = 34 cent/ton, B = 23 cent/ton, and Ss = 336 ppm, the same values adopted from Kim (2012). $C_{\mathrm{ww},n}$ (ppm) and $F_{\mathrm{ww},n}$ (ton/h) are the wastewater contaminant concentration and the wastewater flow rate, respectively. The wastewater charge (CD) is calculated in k\$/yr.

The total annualized cost (CT) consisted of freshwater supply cost (CF), regeneration cost (CR), and waste disposal charge (CD) is formed in Eq. 6.13.

$$\begin{cases} CT_n = CF_n + CR_n + CD_n \\ \forall n \in N \end{cases} \qquad (6.13)$$

Now the optimum post-regeneration concentration is taken as the one which leads to the minimum total cost. Optimization results for the example studied in this paper are discussed in the next section.

6.3.2 Total cost evaluation

All cost functions are plotted against the feasible range of post-regeneration in Figure 6.8. The interaction among cost functions can be vividly observed. The minimum total cost of 506.4 k\$/yr can be determined at 38.3 ppm of optimum post-regeneration concentration ($C_{0\mathrm{opt}}$). Lower than $C_{0\mathrm{opt}}$, the total cost increases with the decrease of C_0 because of the rapidly increasing regeneration cost. Higher than $C_{0\mathrm{opt}}$, wastewater and freshwater costs have the dominant influence in the total cost.

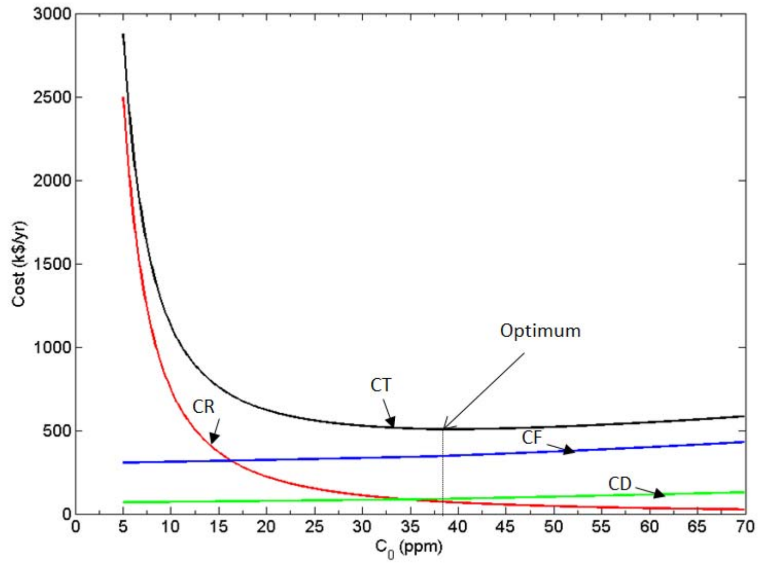

Figure 6.8.Cost function against post-regeneration concentration

Three water network scenarios have been under investigation: maximum reuse (scenario 1), total water regeneration with the specified C_0 (specified RR) (scenario 2), and optimum total water regeneration (scenario 3). Targeting results and cost evaluations are compared in Table 6.1.

Table 6.1.Results comparison for three different scenarios of water network

Scenarios	Maximum reuse/recycle (Chapter 3) Scenario 1	Total regeneration with C_0 =20 (Chapter 5) Scenario 2	Optimum total regeneration (Chapter 6) Scenario 3
Freshwater flow rate (ton/h)	70	37.5	40.2
Wastewater flow rate (ton/h)	50	17.5	20.2
Regenerated water flow rate (ton/h)	-	37.5	40.2
Wastewater concentration (ppm)	200	250	250
Post-regeneration concentration (ppm)	-	20	38.3
Removal Ratio	-	88%	76%
Freshwater cost (k$/yr)	602	322.5	345.7
Wastewater cost (k$/yr)	204.7	76.8	88.6
Regeneration cost (k$/yr)	-	222.6	72.1
Total cost (k$/yr)	806.7	621.9	506.4
Cost saving compare to scenario 1	-	22.9%	37.2%
Cost saving compare to scenario 2	-	-	18.5%

Both scenario 2 and 3 are obviously favourable compared to the maximum reuse/recycle network because of the less demand of freshwater and lower total cost. The optimum case (scenario 3) requires more freshwater, and in turn, generates higher wastewater in contrast with scenario 2. However, the total cost of scenario 3 is lower than the other two. Thus, if economic initiative is the goal, scenario 3 would be the preferred option.

The graphical presentation of the optimum targeting results (scenario 3) is shown in Figure 6.9. The targets obtained for scenario 2 can be referred back to Chapter 5 (Figure 5.2). Since water supply composite curves for both scenarios are located entirely below the LCC, the feasibility of the results is guaranteed. Moreover, the pinch points show the bottleneck of the network.

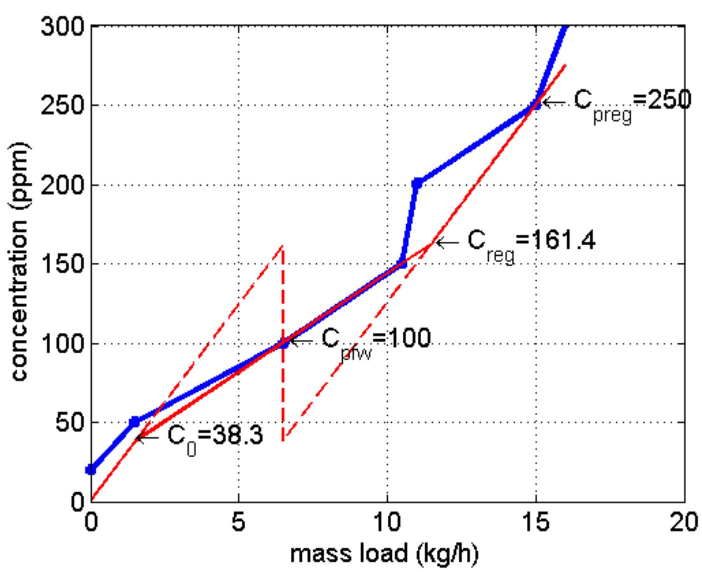

Figure 6.9.LCC and water supply composite curve for the optimum total water regeneration network (scenario 3)

Figure 6.10 gives one possible network design for optimum scenario (scenario 3) as a matching matrix.

		F_{SKj} (ton/h)	50	100	80	40.2	70	20.2
		C_{SKj} (ppm)	20	50	100	161.4	200	250
F_{SRi} (ton/h)	C_{SRi} (ppm)	SR*i* \ SK*j*	SK1	SK2	SK3	Regin	SK4	WW
40.2	0	FW	23.9	16.3				
40.2	38.3	Regout	26.1	14.1				
50	50	SR1		50				
100	100	SR2		19.6	80		0.4	
70	150	SR3				35.6	34.4	
60	250	SR4				4.6	35.2	20.2

Figure 6.10.Water Network Design for scenario 3 as a matching matrix

In comparison with the network design for the second scenario (Figure 5.3), the forbidden matches region is changed due to the different pinch point location. Higher freshwater and regenerated water flow rate are required. SR3 and SR4 feed the regeneration unit to be purified for further reusing in SK1 and SK2. As demonstrated, all the targets are satisfied through network synthesis

6.4 Cost sensitivity analysis

The cost evaluation definitely depends on the unit cost used for the optimization study. The total water regeneration network has an economic justification over the maximum reuse/recycle system when the regeneration cost is relatively lower than freshwater supply cost and waste disposal charge (Feng and Chu, 2004). The regeneration cost has the dominant influence to the total cost of the system as presented in Figure 6.8. Thus, the unit cost of regenerator (α) is chosen for analysis. By incrementally increasing ALPHA (α) between 1 and 143, the trade-off between ALPHA (α), C_{0opt}, and the amount of saving for optimum scenario compared with reuse/recycle scheme (saving-opt-reuse) is demonstrated in Figure 6.11. Several valuable insights can be reported through this analysis. Firstly, it is observed that by increasing α while C_{0opt} is increasing, the cost saving is declining meaning that the network moves toward the maximum reuse/recycle scheme. Secondly, as shown, C_{0opt} is sharply increasing for the range of α between 1 and 9. This targets the highly sensitive region for optimization study. Two neutral regions are fond for α from 1 to 9 and 117 to 143 with the constant C_{0opt} of 37.5 ppm and 69.9 ppm. The C_{0opt} is slightly increasing for the range of α between 13 and 117. This region shows the low sensitive region. Thirdly, as mentioned, cost saving for optimum scenario is declining with the increased contribution of regeneration cost to the total cost. With reaching to the α of 143 equated to regeneration cost of 248 k$/yr, there would be no more economic beneficial to implement total water regeneration scheme. The cost of optimum regeneration scenario lies on the maximum reuse/recycle scheme. Therefore, one will choose maximum reuse/recycle scheme as the preferred option.

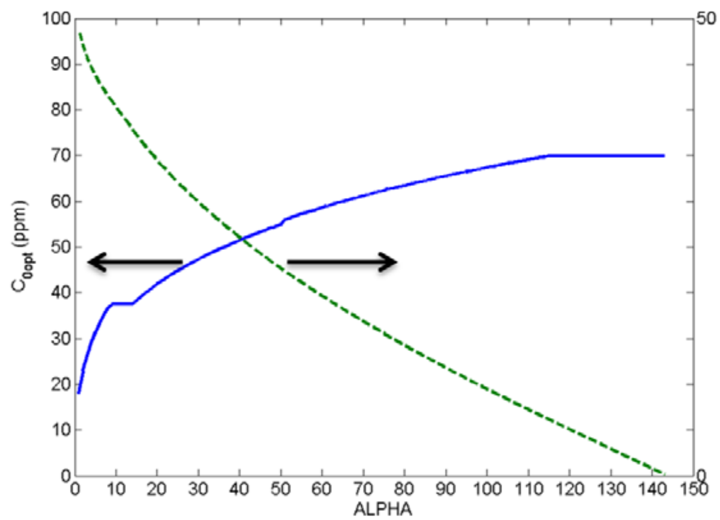

Figure 6.11.Trade-off between ALPHA (α), C_{0opt}, and cost saving for optimum scenario compared with reuse/recycle scheme

6.5 Summary

The new targeting method, CMA, is proposed by systematically relaxing the assumption of fixed-post regeneration concentration. This method provides the key parameters in total regeneration water network considering RR criterion which was lagged behind before. Several valuable insights also have been reported such as pinch migration, and minimum feasible regeneration performance. Since the post-regeneration concentration has the dominant influence to the total cost of the system, by relaxing this parameter, the economic evaluation is conducted. Most of WPA studies considered the lower the post regeneration concentration as the better option due to higher pure utility saving. However, this study reveals that this issue cannot guarantee the economic optimality and the economic optimum scenario has been set up by applying CMA as a tool.

7. WATER UTILISES MINIMIZATION FOR THRESHOLD PROBLEMS WITHOUT WASTE DISCHARGE

As introduced in Chapter 4, "Threshold Problems" in the water network synthesis are rare but realistic where the network requires either fresh water feed without waste disposal or generates waste water without fresh water intake. In an even special situation, the network may neither require fresh water feed nor encounter waste discharge.

Threshold problems in the FF model initially were addressed by WCA and MRPD (Foo, 2008). Later, Alwi and Manan (2007) extended MRPD approach to target the flow rates of utilities for the "threshold problem without water discharge". For this case, the feasible process pinch point does or does not exist. If the feasible process pinch point does not exist, three different scenarios can be applied to recover the feasibility of the problem by using external utilities. These scenarios are: (1) to utilize more pure fresh water source; (2) to employ the external utility below an infeasible process pinch point; (3) to use an external utility above the infeasible pinch point. The first scenario was addressed using both WCA and MRPD (Foo, 2008). The second scenario was implemented via MRPD (Alwi and Manan, 2007). In this work, the use of external utility above infeasible pinch point is going to be adopted to deal with the infeasible threshold problem.

Prior to recovering the feasibility, it is thought important to find infeasible targets (fresh water flow rate, waste water flow rate, and the pinch point) first. In order to do so, some adjustments are necessary for the existing WCA method to locate those infeasible targets. In addition, both WCA and MRPD targeting techniques can be utilised as complementary tools to locate minimum external utilities flow rate in these scenarios. The new contribution that has emerged from this work is to provide a new physical insight to the "threshold problem without waste discharge", that is, to reduce the pure fresh water in favour of the external impure utility. In the "threshold problem without water discharge" regeneration (Chapters 5 & 6) cannot provide fresh water saving solution because of insufficient water sources. Thus, it can be argued that the best option for saving fresh water in this case is harvesting the external impure water source.

In this chapter, after the problem statement, different types of threshold problems will be explained through source-sink composite curves. Based on this, three different scenarios will be proposed for harvesting the external utility in the "threshold problem with zero discharge". Then, a literature example will be addressed by utilizing both MRPD and WCA approaches under the proposed scenarios before concluding remarks.

7.1 Problem statement

The superstructure presentation of the problem is depicted in Figure 7.1.

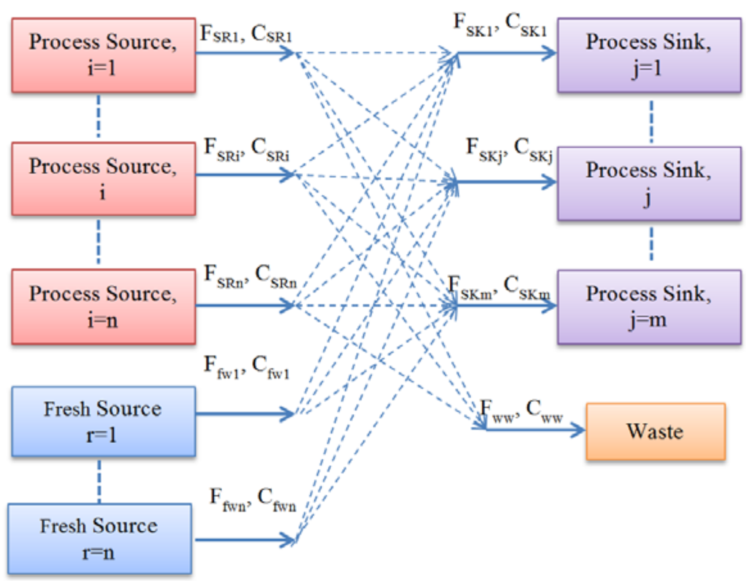

Figure 7.1.Source/sink presentation of reuse/recycle water network with multiple utilities

Consider a process that includes a set of process sinks and a set of process sources:

- Processes needing water are designated as Process Sinks or SKj (j=1, 2, … m). Each sink has a given flow rate, F_{SKj} and inlet concentration, C_{SKj}, which must satisfy: $C_{SKj}^{min} \leq C_{SKj} \leq C_{SKj}^{max}$, where C_{SKj}^{min} and C_{SKj}^{max}, is the lowest and the highest of concentration limit.

- Water-generating processes, which are reused or recycled to Process Sinks are designated as Process Source, or SR*i* (i= 1, 2,…, n), with a given flow rate of F_{SRi}, and an impurity concentration of C_{SRi}.
- If Process Sources cannot satisfy Process Sinks, the external freshwater source(s) (r=1,2, …,n) with specific concentration (C_{fw}) is introduced to fulfil the requirement of the sinks flow rate. Unused water from process sources (if any) will be directed to the waste with the concentration of (C_{ww}) and the flow rate of (F_{ww}).

Given the above-described process, the objective is to provide the new conceptual view to the "threshold problem with zero discharge" in the water network synthesis for minimizing the flow rate of fresh water source(s).

Not all problems in the water network synthesis encounter the fresh water consumption and the waste discharge concurrently. This type of problem is termed as the "threshold problem" (Foo, 2008). Similar concept is also introduced in a heat exchanger network synthesis where a network needs either cold utility or hot utility (Kemp, 2007; Smith, 2005). In water network synthesis, the threshold problem falls in to three categories, i.e. zero network discharge with fresh water feed (Figure 7.2a), network generates waste without fresh water feed (Figure 7.2b), and network with no fresh water and zero discharge (Figure 7.2c). These three categories can be easily distinguished by the source-sink composite curve (Figure 7.2).

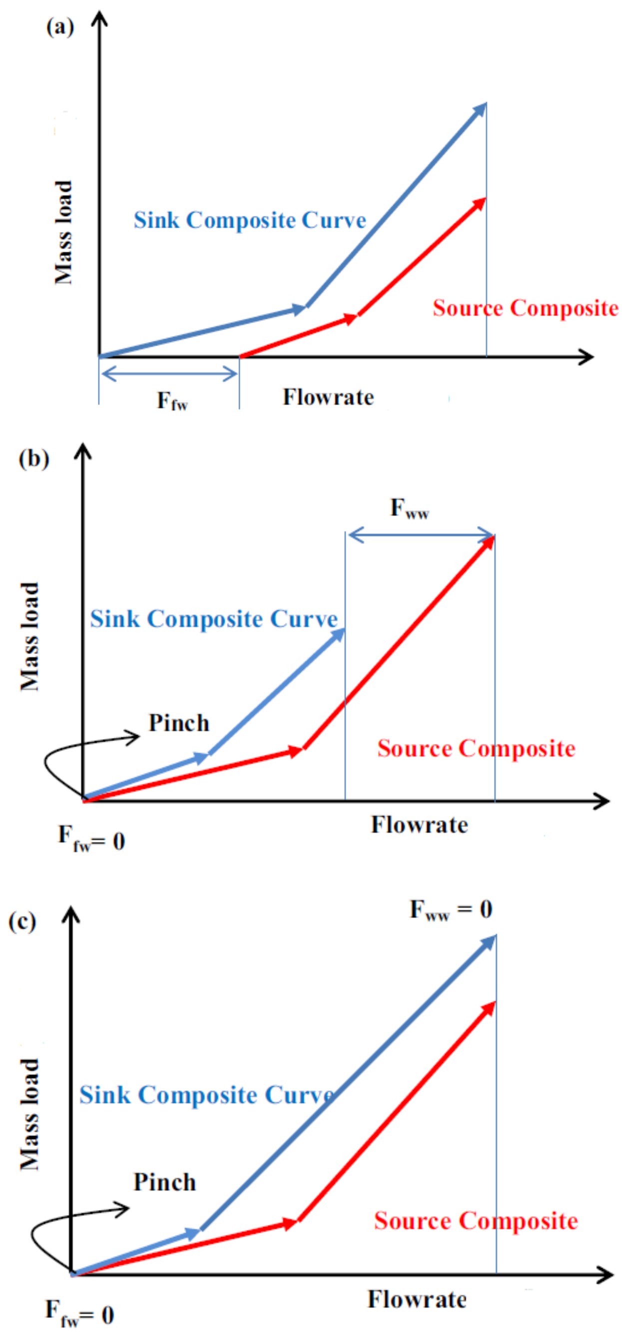

Figure 7.2.Three categories of threshold problem: (a) zero network discharge; (b) network without fresh water feed; (c)network with zero fresh and waste water

To describe some specific features of the threshold problem, it is essential to briefly recap the flow rate targeting procedure in MRPD method (Chapter 3). Initially, the source and sink composite curves are constructed on the flow rate and mass load diagram from origin (zero flow rate and mass load (Figure 7.3a). Then source composite curve is shifted horizontally until it is located entirely to the right of the sink composite curve and touches the latter at the pinch point (Figure 7.3b). Having identified the pinch point, the overhang below and above the pinch point determines the fresh water flow rate (F_{fw}) and the waste water flow rate (F_{ww}) targets respectively. Note that the pinch locates always at one of the source qualities and this particular process source known as the pinch-causing source.

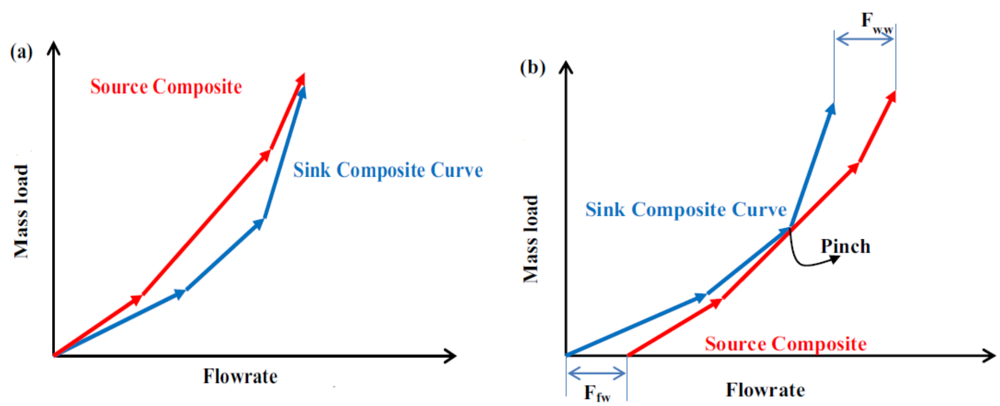

Figure 7.3.Flow rate targeting procedure in MRPD method: (a) source–sink composite curves and (b) pinched source–sink composite curves

Applying MRPD technique for flow rate targeting in the threshold problem is not the same as for general water network synthesis problems. As shown in Figure 7.2b & c, the source composite curves in these two cases are already below the sink composite curves. Therefore, there is no need to further move the source composite to the right to ensure the contaminant load feasibility. As described in Chapter 4, dissimilar to the normal water network problem, the pinch point is located at the lowest source concentration and there is no need for fresh water feed. The horizontal difference between source and sink composite curves in the right end identifies the waste flow rate target. Although, for the case shown in Figure 7.2b, there is an excess flow rate of process sources which has not been used in the process sinks, for the case in Figure 7.2c, all flow rates in the process sources has been utilized in the process sinks after reuse/recycle has taken place.

Figure 7.2a is the only case which requires fresh water feed. There is an opportunity here to reduce pure fresh feed by introducing the impure utility. The same work was also done in the heat exchanger network problem by introducing the second utility (Smith, 2005). Alwi and Manan (2007) demonstrated that graphical MRPD method can be applied for multiple utilities in the water network synthesis. They also used this approach to utilize the impure water source in the "threshold problem without waste discharge". However, there are two ways of using impure fresh water source, below or above the pinch-causing source. The extended MRPD approach (Alwi and Manan, 2007) only used the impure fresh water source below the pinch without considering the one above the pinch.

In the following, different scenarios for using external utility in the threshold problem without waste discharge will be discussed. Moreover, it will be shown that, with some adjustment, WCA approach can also handle this kind of problem. WCA method provides numerical accuracy and, therefore, complements the work done earlier (Alwi and Manan, 2007).

7.2 Threshold problem infeasibility and recovery strategies

For systematically harvesting external utility in the threshold problem without waste discharge, the following important points need to be noticed.

Similar to the general MRPD targeting procedure, after constructing the source and sink composite curves, the source composite curve is moved horizontally closer to the sink composite satisfying the mass load constraint. During this process, these two composites touch each other at the pinch point. However, two different results may occur here. In one case, both of the composite curves are in alignment at the right end (Figure 7.4a). This means that, the network encounters zero waste discharge and the minimum fresh water flow rate target has already been achieved. For the other case, the total available sources are insufficient for the sinks (Figure 7.4b). Hence, the external fresh water source is required to supplement the fresh water flow rate shortage. The evidence is the negative waste water flow rate above the pinch quality. We call this problem and its pinch quality as the "Infeasible Threshold Problem" and "Infeasible Threshold Pinch Point (ITPP) Concentration, respectively.

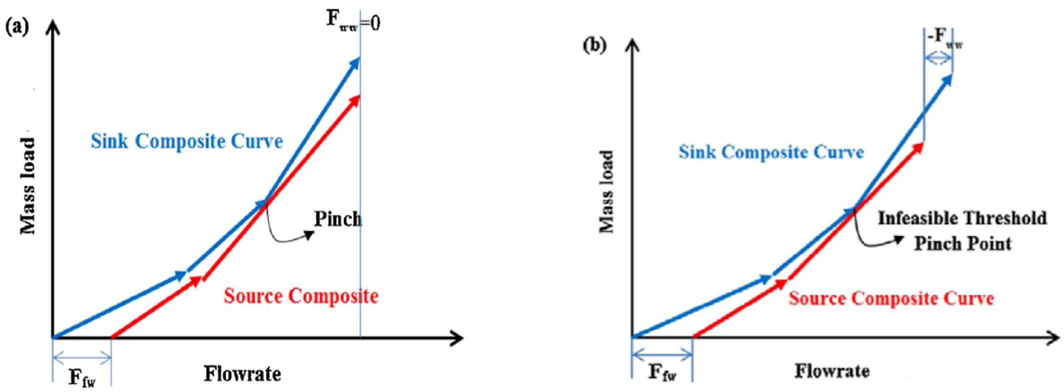

Figure 7.4.Threshold problem without waste discharge: (a) feasible and (b) infeasible

For the "Infeasible Threshold Problem", three scenarios can be applied using the external water source to recover the feasibility of the problem, namely:

(1) To employ more pure fresh water source;

(2) To harvest the impure utility with the concentration lower than the pinch-causing source (Lower than ITPP); and

(3) To use the impure water source which is dirtier than the pinch-causing source (higher than ITPP).

Under the first scenario, utilizing more pure fresh water moves the source composite curve further to the right until it comes in alignment with sink composite at the right end. Numerically, summing up the fresh water (F_{fw}) and the absolute negative waste water (F_{ww}) flow rates at both ends of MRPD diagram leads to the minimum fresh water flow rate target. By doing so, the ITPP will disappear; the fresh water flow rate will be increased, and the infeasible waste water flow rate will be eliminated. This scenario has been addressed by Foo using MRPD and WCA methods (Foo, 2008). The final source-sink composite curves of this scenario are depicted in Figure 7.2a earlier.

In the other two scenarios, employing the impure utility provides more room for fresh water saving. The introduction of second utility under the pinch-causing source will generate a new utility pinch point and the ITPP will disappear (Figure 7.5a). Under this situation, the fresh water flow rate (F_{fw}) will be reduced along with setting the source composite curve in alignment with the sink composite curve in the right end. This means that the pure fresh water flow rate (the highest quality water source) will be reduced in favour of the lower quality water source. At the same time, the waste water flow rate infeasibility will be resolved. This scenario has been addressed by Alwi and Manan (2007) using MRPD method as a targeting tool. Introduced impure utility is indicated with dashed line in Figure 7.5a and its flow rate target (F_{ifw}) is set as a projection of horizontal distance on the flow rate axis. In this work, numerical WCA method with minor adjustment will be applied to complement the graphical MRPD method. Moreover, it will be demonstrated that the higher quality impure fresh water source will provide more opportunity to save the pure fresh water source.

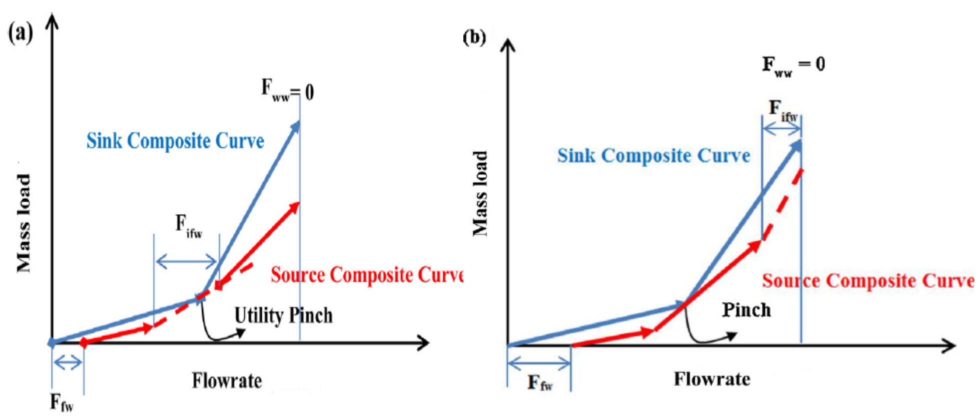

Figure 7.5.Schematic diagram for introducing impure utility in the threshold problem without waste discharge: (a) utility below the ITPP and (b) utility above the ITPP.

In the third scenario, the ITPP location and the original fresh water flow rate (F_{fw}) target will not be changed (Figure 7.5b). However, adding the impure utility with the concentration higher than the pinch-causing source recovers the feasibility of the problem. The shortage of water flow rate is satisfied with the introduction of the impure utility above the pinch point. The impure utility flow rate (F_{ifw}), numerically, is the absolute value of the negative waste water flow rate

(F_{ww}). Although the ITPP location has not been changed, its name will be replaced by Pinch concentration after the problem infeasibility is eliminated.

It has been shown that harvesting the impure water source with a higher quality, in the threshold problem with zero discharge, leads to more pure fresh water saving (This will be quantified later through an illustrative example). However, the purer the water source is, the more expensive it is. Hence, to find the best scenario for using the external utilities in this particular problem, the optimization should be considered. The concept of prioritised cost proposed by Shenoy and Bandyopadhyay (2007) may be helpful to find the economic optimum option. Economic evaluation of this problem can be considered as a future studies.

For systematically addressing flow rate targeting of the utilities, ITPP plays a key role. Therefore it is necessary to locate the ITPP correctly before applying the proposed scenarios. Using an illustrative example, we will explain that general WCA method (described in Chapter 3) cannot correctly locate the infeasible threshold targets. This approach, therefore, needs some adjustments. Moreover, the proposed scenarios for external utility targeting will be considered using both WCA and MRPD methods.

7.3 Utilities targeting for Infeasible Threshold Problem

Table 7.1 shows the limiting water data for an illustrative example (Foo, 2008). There are three process sources which can be reused/recycled to the three process sinks. Before applying reuse/recycle, the network consumes 170 ton/h of fresh water and also generates 110 ton/h of waste water.

Table 7.1.Limiting water data(Foo, 2008)

Sink	F_{SKj} (ton/h)	C_{SKj} (ppm)	Source	F_{SRi} (ton/h)	C_{SRi} (ppm)
SK1	50	20	SR1	20	20
SK2	20	50	SR2	50	100
SK3	100	400	SR3	40	250
Total	170		Total	130	

Fresh and waste water flow rates as well as pinch concentration for reuse/recycle network can be targeted by either algebraic methods such as WCA or graphical approaches such as MRPD. Using WCA and MRPD techniques, the resulting infeasible targets are listed in Table 7.2.

Table 7.2.Infeasible targets for reuse/recycle network

Methods	Freshwater flow rate F_{fw} (ton/h)	Wastewater flow rate F_{ww} (ton/h)	ITPP concentration
WCA	59.97	-0.03	1,000,000
MRPD	34	-26	100

As seen, ITPP concentration from WCA locates on the highest allowable concentration (1 million ppm). This value is not among any of the sink or source concentration. As described in Chapter 3, this contaminant concentration is added in the first column of Water Cascade Table (WCT) to facilitate the interval impurity load cascading in the later stage of general WCA method. In addition, the fresh water and the infeasible waste water flow rate targets are 57.97 (ton/h) and -0.03 (ton/h) respectively. On the other hand, by applying MRPD approach, the ITPP concentration target is located on SR2 concentration. The fresh water and the infeasible waste water flow rate targets are determined as 34 ton/h and -26 ton/h.

Since, MRPD approach provides physical insight due to its graphical characteristic, the targets obtained by MRPD approach are deemed more reliable than that determined by WCA method. From this point, applying general WCA method for this kind of problem in water network synthesis cannot correctly locate the infeasible targets. Moreover, our earlier discussion revealed that ITPP concentration provides physical insight for harvesting external water source and should be located correctly before recovering the feasibility of the problem through introducing external utility. To overcome this drawback, an adjustment is necessary for the generic WCA approach so that it can adapt to this particular problem. This is described below.

In the first step of WCA method, eliminate one million ppm concentration at the end of column 2 from analysis and follow the same procedure as described earlier in Chapter 3. With this adjustment, WCA technique produces exactly the same targets as that from MRPD approach. This is illustrated in the modified WCT (Table 7.3).

Table 7.3.Modified WCT- Infeasible flow rate cascade

1	2	3	4	5	6	7	8
k	C_k (ppm)	$S.F_{SKj}$ (ton/h)	$S.F_{SRi}$ (ton/h)	$S.F_{SRi}$- $S.F_{SKj}$ (ton/h)	$F_{c,k}$ (ton/h)	Δm_k (kg/h)	Cum. Δm_k (kg/h)
1	0				$\boldsymbol{F_{fw}}$**= 34**	0.68	
2	20	50	20	-30	4	0.12	0.68
3	50	20		-20	-16	-0.8	0.8
4	100		50	50	34	5.1	0 (ITPP)
5	250		40	40	74	11.1	5.1
6	400	100		-100	$\boldsymbol{F_{ww}}$**=-26**		16.2

The ITPP locates on 100 ppm concentration associated to the zero cumulative mass load. As all cumulative mass load values in column 8 are zeroes or higher, the existing fresh water flow rate satisfies the impurity mass load constraint. However, flow rate cascading in column 6 indicates a negative waste water flow rate for the network. Hence, this amount of fresh water cannot meet the flow rate constraint of the model.

In the following, three different scenarios will be applied to fulfil the flow rate constraint and to resolve the infeasibility of the problem. Under the second scenario, two different cases will be taken into account. In case 1, impure utility with 40 ppm contaminant concentration is considered while for case 2, it is supposed that water source at 30 ppm contaminant concentration serves the network.

We will address these scenarios by utilizing WCA and MRPD approaches as the targeting tools.

7.3.1 Scenario 1: The introduction of more pure fresh water source

The first scenario is to employ more pure fresh water. Numerically, the absolute flow rate of infeasible waste water (F_{ww}=26 ton/h) and fresh water (F_{fw}=34) are added together to give the feasible fresh water flow rate target of 60 ton/h. The final WCT with the revised flow rate cascading is illustrated in Table

7.4 while the final source-sink composite curves are shown in Figure 7.6. The ITPP is removed due to the addition of fresh water and no pinch-causing source can be found in this scenario. Last concentration level (400 ppm) is known as threshold concentration.

Table 7.4.Final WCT-feasible flow rate cascading for scenario 1

1	2	3	4	5	6	7	8
k	C_k (ppm)	S.F_{SKj} (ton/h)	S.F_{SRi} (ton/h)	S.F_{SRi}- S.F_{SKj} (ton/h)	$F_{c,k}$ (ton/h)	Δm_k (kg/h)	Cum. Δm_k (kg/h)
1	0			0	$\boldsymbol{F_{fw} = 60}$	1.2	
2	20	50	20	-30	30	0.9	1.2
3	50	20		-20	10	0.5	2.1
4	100		50	50	60	9	2.6
5	250		40	40	100	15	11.6
6	400	100		-100	$\boldsymbol{F_{ww} = 0}$		26.6

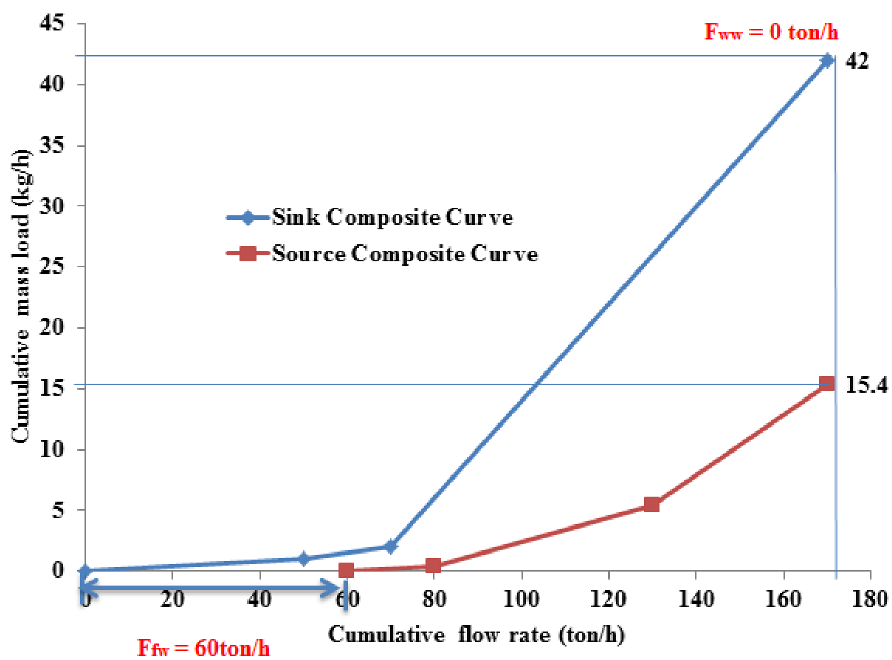

Figure 7.6.Source–sink composite curves for scenario 1

It is worth mentioning that the final targeting result for this scenario is the same as in Foo (2008). CTA was utilised to address this scenario in Chapter 4 (Example 4.4) and the same targets were reported. In addition, one possible water allocation network was constructed employing NNA in Chapter 4 (Figure 4.8).

7.3.2 Scenario 2: The introduction of impure utility with concentration lower than ITPP

A higher quality water source is usually more valuable. Using the impure utility below the ITPP provides more space to reduce the pure fresh water source. It is worth mentioning that the impure fresh water source with lower concentration (cleaner impure water source) is preferred when different water sources with different qualities are available for service. Using the higher quality water source in this kind of problem would have less demand for the pure utility. One may make an assumption here that the impure utility is virtually cost free compared to the pure utility. As mentioned, this assumption may be relaxed through the prioritised cost function (Shenoy and Bandyopadhyay, 2007).

For the presence of multiple utilities with different concentrations, the modified procedure of WCA is required which was described in Chapter 3. A three-step approach to target the minimum flow rate for each utility is recapped as follows:

Step 1: Identify the flow rate for the lower quality water source.

Step 2: Determine the flow rate for the higher quality water source.

Step 3: Adjust the flow rate for the lower quality water source.

To demonstrate that using the higher quality impure water source provides more room for the pure fresh water saving, two different cases are examined.

Case 1: Freshwater and impure utility with 40 ppm contaminant concentration

For case 1, consider the impure fresh water source with 40 ppm concentration available for service along with the pure utility. By conducting WCA with the proposed modification in this research, the WCT after the flow rate adjustment for the lower quality water source (Step 3 as stated above) is depicted in Table 7.3. All values with respect to cumulative mass loads (Cum.Δm_k) in the column 8 are zero or positive. This means that the total flow rate of pure and impure water sources satisfies the mass load constraint. However, there is an infeasible negative waste water flow rate which indicates the total water serving the network is not fulfilling the flow rate constraint.

Table 7.5.WCT after flow rate adjustment for the lower quality water source with 40 ppm concentration -infeasible flow rate cascading (scenario 2-case 1)

1	2	3	4	5	6	7	8
k	C_k (ppm)	S.F_{SKj} (ton/h)	S.F_{SRi} (ton/h)	S.F_{SRi}- S.F_{SKj} (ton/h)	$F_{c,k}$ (ton/h)	Δm_k (kg/h)	Cum. Δm_k (kg/h)
1	0			0	$\boldsymbol{F_{fw}}$**= 15**	0.30	
2	20	50	20	-30	-15	-0.30	0.30
3	<u>40</u>		$\boldsymbol{F_{ifw}}$ **= 31.67**	31.67	16.67	0.17	0 (Utility pinch)
4	50	20		-20	-3.33	-0.17	0.17
5	<u>100</u>		50	50	46.67	7.00	0 (ITPP)
6	250		40	40	86.67	13.00	7.00
7	400	100		-100	$\boldsymbol{F_{ww}}$ **= -13.33**		20.00

This infeasibility can be resolved readily by adding the absolute value of waste water flow rate (F_{ww}) to the impure fresh water flow rate (F_{ifw}). The revised WCT after recovering the flow rate feasibility is shown in Table 7.6.

Table 7.6.Revised WCT with feasible flow rate cascading for scenario 2-case 1

1	2	3	4	5	6	7	8
k	C_k (ppm)	S.F_{SKj} (ton/h)	S.F_{SRi} (ton/h)	S.F_{SRi}- S.F_{SKj} (ton/h)	$F_{c,k}$ (ton/h)	Δm_k (kg/h)	Cum. Δm_k (kg/h)
1	0			0	$\boldsymbol{F_{fw}}$ **= 15**	0.30	
2	20	50	20	-30	$\boldsymbol{F_{ifwbp}}$ **=-15**	-0.30	0.30
3	<u>40</u>		$\boldsymbol{F_{ifw}}$ **= 45**	45	$\boldsymbol{F_{ifwap}}$ **=30**	0.30	0 (Utility pinch)
4	50	20		-20	10	0.50	0.30
5	100		50	50	60	9.00	0.80
6	250		40	40	100	15.00	9.80
7	400	100		-100	$\boldsymbol{F_{ww}}$ **= 0**		24.80

Revising flow rate cascading results in pure (F_{fw}), impure (F_{ifw}), and waste water flow rates (F_{ww}) to be 15 ton/h, 45 ton/h and 0 ton/h. Compared to scenario 1, the use of impure utility will save the pure fresh water usage by 75%, although total amount of required utility (60 ton/h) remains the same. The ITPP is removed, and the new utility pinch is introduced at 40 ppm concentration. One other specific feature of the feasible WCT is the flow rate allocation of the impure utility across the pinch point. These flow rate allocations can be easily found from the below (F_{ifwbp}= 15 ton/h) and the above (F_{ifwap}= 30 ton/h) of the pinch point in the 6th column. All these targets also can be found by using MRPD targeting technique. For locating the true targets the proposed procedure in reference (Alwi and Manan, 2007) should be followed. The final source-sink composite curves applying MRPD method are depicted in Figure 7.7.

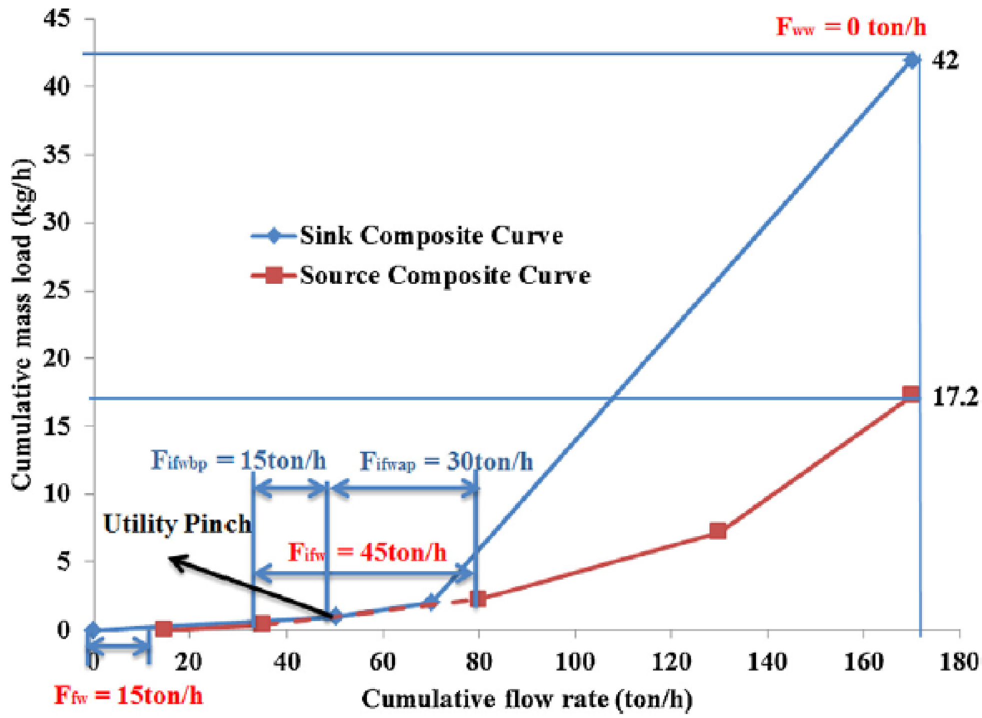

Figure 7.7.Source–sink composite curves for scenario 2 – case1

It is worthy to note that introducing impure utilities for the normal pinch problem cause higher total utility requirement and wastewater generation (see Chapter 3, section 3.1.2 for more information). However, as demonstrated, the total utility requirement for the threshold problem does not change with the introduction of impure utility.

Network design is formed as matching matrix utilising NNA in Figure 7.8. In contrast with scenario 1, this network has forbidden matches regions due to appearance of utility pinch point. The process sinks are satisfied with the ascending order of contaminant concentrations.

		F_{SKj} (ton/h)	50	20	100
		C_{SKj} (ppm)	20	50	400
F_{SRi} (ton/h)	C_{SRi} (ppm)	SK*j* / SR*i*	SK1	SK2	SK3
15	**0**	**FW**	15		
20	20	SR1	20		
45	**40**	**IFW**	15	16.67	13.33
50	100	SR2		3.33	46.67
40	250	SR3			40

Figure 7.8.Network design as a matching matrix for scenrio2- case 1

The impure freshwater utility (IFW) is considered as one of the process sources and arranged based on the increasing order of concentration. Therefore, it should be located after SR1 with contaminant concentration of 20 ppm. Together with the other targets, the flow rate allocation targets of impure utility are also achieved through the network design. 15 ton/h of impure utility is utilised for SK1 located below the pinch and the remaining flow rate is exhausted for SK2 and SK3 placed above the pinch point. The same as other threshold problems (described in Chapter 4), although the flow rate of lowest quality process sink (SK3) is satisfied, its total mass contaminant load cannot be picked up.

Case 2: Freshwater and impure utility with 30 ppm contaminant concentration

For case 2, it is assumed that the pure fresh water and the impure fresh water with 30 ppm concentration are available for service. The WCT after recovering the flow rate feasibility is shown in Table 7.7 and the final source-sink composite curves are also depicted in Figure 7.9.

Table 7.7.Revised WCT with feasible flow rate cascading for scenario 2- case 2

1	2	3	4	5	6	7	8
k	C_k (ppm)	S.F_{SKj} (ton/h)	S.F_{SRi} (ton/h)	S.F_{SRi}- S.F_{SKj} (ton/h)	$F_{c,k}$ (ton/h)	Δm_k (kg/h)	Cum. Δm_k (kg/h)
1	0			0	$\boldsymbol{F_{fw}}$ **= 10**	0.2	
2	20	50	20	-30	$\boldsymbol{F_{ifwbp}}$ **=-20**	-0.2	0.2
3	<u>30</u>		$\boldsymbol{F_{ifw}}$ **= 50**	50	$\boldsymbol{F_{ifwap}}$ **= 30**	0.6	0 (Utility pinch)
4	50	20		-20	10	0.5	0.6
5	100		50	50	60	9	1.1
6	250		40	40	100	15	10.1
7	400	100		-100	$\boldsymbol{F_{ww}}$ **= 0**		25.1

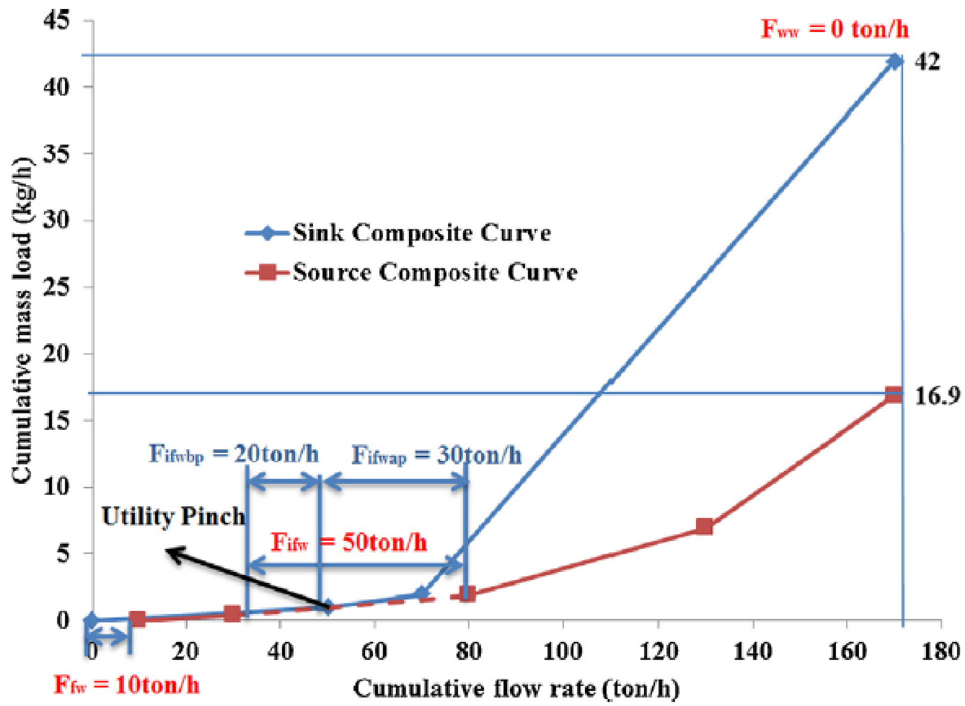

Figure 7.9.Source–sink composite curves for scenario 2 – case2

The fresh water flow rate target is reduced by 5 ton/h (33 precent) compared with case 1. On the other hand, the flow rate of impure utility with 30 ppm concentration is higher than that with 40 ppm concentration. This means that the cost of impure utility is increased but, the need for pure water source (the highest quality water source) is decreased (compare to case 1). Hence, to find the best optimum results, the trad-off between these parameters should be considered. Some works have addressed cost factors in multiple water sources case applying pinch analysis (Deng and Feng, 2011; Foo, 2012; Shenoy and Bandyopadhyay, 2007). However, as mentioned, the main scope of this work is providing the physical insight for water saving in the "threshold problem with zero discharge" without taking into account of the optimum cost.

Network design for this case following NNA procedure is also illustrated in Figure 7.10. All the targets are achieved in practice.

		F_{SKj} (ton/h)	50	20	100
		C_{SKj} (ppm)	20	50	400
F_{SRi} (ton/h)	C_{SRi} (ppm)	SKj / SRi	SK1	SK2	SK3
10	**0**	**FW**	10		
20	20	SR1	20		
50	**30**	**IFW**	20	14.29	15.71
50	100	SR2		5.71	44.29
40	250	SR3			40

Figure 7.10.Network design as a matching matrix for scenrio2- case 2

7.3.3 Scenario 3: The use of impure water source with concentration higher than ITPP

As discussed in the previous section, using the impure water source above the pinch-causing source (SR2 with 100 ppm concentration) will not change the ITPP location and also cannot reduce the amount of infeasible pure fresh water source (34 ton/h) shown in Table 7.3. However, the shortage of water flow rate above the ITPP can be complimented by external water sources. The flow rate of the external utility will be the absolute value of negative waste water flow rate (26 ton/h). As the flow rates of impure and pure water sources will not be changed, hence, harvesting the dirtiest possible utility is the preferred option. Using dirtier water source means the lower operating cost. However, it has to be noted that the concentration of this utility is limited by the lowest quality process sink.

MRPD approach is adopted as the targeting tool to address how the lowest quality water sink dictates the maximum possible concentration of the impure utility. Source composite curve should always be at right and below the sink composite curve. In addition, the slope of each segment for sink and source composite curves identifies the contaminant concentration. The source-sink composite curves before resolving the infeasibility of the problem are shown in Figure 7.11.

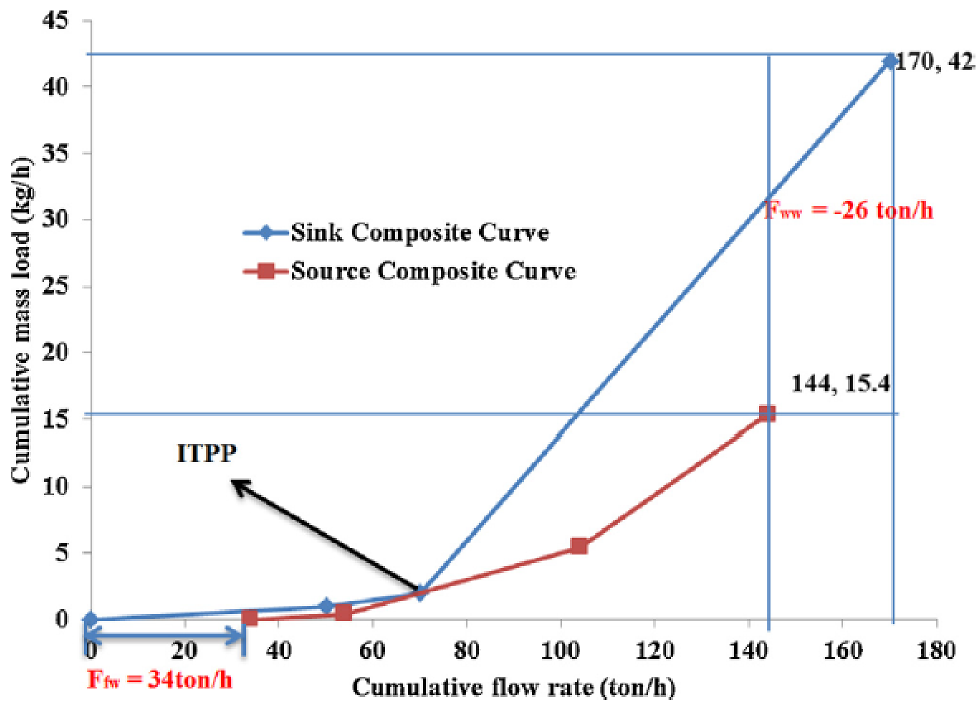

Figure 7.11.Infeasible source–sink composite curves

The lowest quality water sink (SK3 with 400 ppm concentration, 100 ton/h flow rate) in the last segment of the sink composite curve ends at the cumulative flow rate of 170 ton/h and the cumulative mass load of 42 kg/h. By adding the lowest quality impure water source above the ITPP, another segment will be introduced to the source composite curve (Figure 7.12).

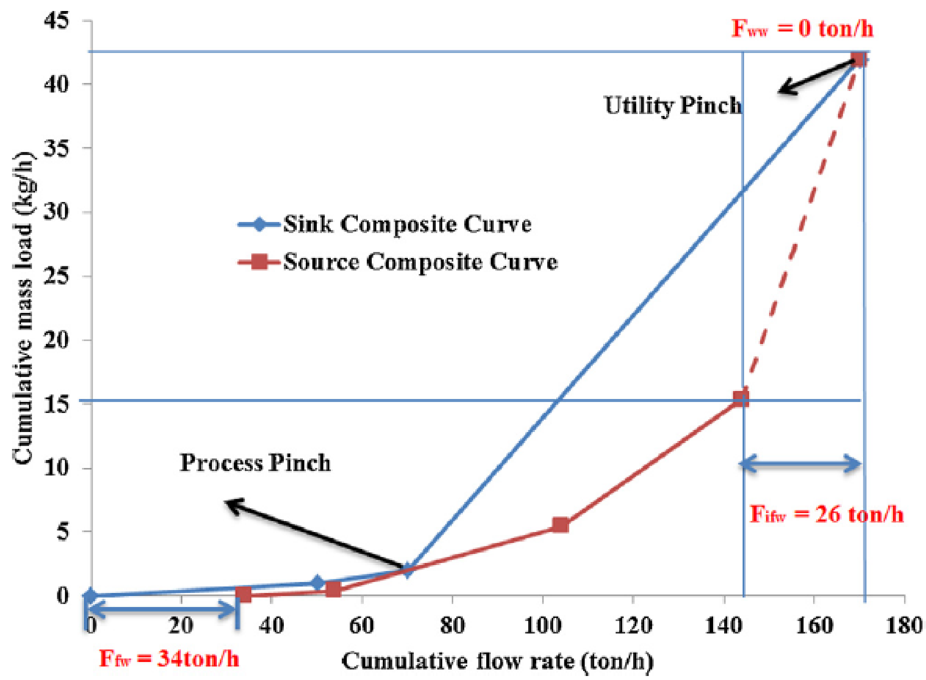

Figure 7.12.Introducing the lowest quality water source for recovering the feasibility of the problem (scenario 3)

This segment should be introduced in a way that, the final source composite curve does not locate to the right and/or above the sink composite curve. In other words, the impure water utility line will be drawn from the end of source composite curve (cumulative flow rate of 144 ton/h and cumulative mass load of 15.4 kg/h) to the end of sink composite curve. The slope of this segment dictates the so called Threshold Maximum Permissible (TMP) concentration of impure utility which can serve the network. This contaminant concentration is identified as 1023 ppm. Introducing any impure utility with flow rate of 26 ton/h and the concentration between 100 ppm (ITPP) and 1023 ppm (TMP) can recover the feasibility of the problem. However, the higher concentration of the impure utility, the lower the operating cost may be achieved. For cases where several water utilities are in use (with similar unit costs), cost calculation needs to be performed in order to find the lowest operating cost. Applying the concept of prioritized cost originally developed by Shenoy and Bandyopadhyay (2007) may be helpful in these cases.

WCA method is also can be applied to set the TMP contaminant concentration target and impure fresh water flow rate for the third scenario. 0 ppm TMP concentration is assumed and added as the last entry to the infeasible WCT (Table 7.3). Following the procedure of general WCA method described in Chapter 3 produces infeasible WCT for third scenario in Table 7.8. The negative wastewater flow rate (-26 ton/h) is found in the last entry of column 6

Table 7.8.Infeasible water cascade table for scenario 3

1	2	3	4	5	6	7	8
k	C_k (ppm)	S.F_{SKj} (ton/h)	S.F_{SRi} (ton/h)	S.F_{SRi}- S.F_{SKj} (ton/h)	$F_{c,k}$ (ton/h)	Δm_k (kg/h)	Cum. Δm_k (kg/h)
1	0				$\boldsymbol{F_{fw}}$**= 34**	0.68	
2	20	50	20	-30	4	0.12	0.68
3	50	20		-20	-16	-0.8	0.8
4	100		50	50	34	5.1	0 (ITPP)
5	250		40	40	74	11.1	5.1
6	400	100		-100	-26	10.4	16.2
7	0 (TMP)			0	$\boldsymbol{F_{ww}}$**=-26**		26.6

26 ton/h of any utility with the contaminant concentration higher than ITPP (100 ppm) can resort the feasibility of the problem. This value is added under sources column (column 4) corresponding with the assumed TMP concentration (Table 7.9). Recovering problem feasibility, ITPP is replaced by Process Pinch.

Table 7.9.Feasible water cascade table including impure freshwater flow rate target for scenario 3

1	2	3	4	5	6	7	8
k	C_k (ppm)	S.F_{SKj} (ton/h)	S.F_{SRi} (ton/h)	S.F_{SRi}- S.F_{SKj} (ton/h)	$F_{c,k}$ (ton/h)	Δm_k (kg/h)	Cum. Δm_k (kg/h)
1	0				$\boldsymbol{F_{fw}}$**= 34**	0.68	
2	20	50	20	-30	4	0.12	0.68
3	50	20		-20	-16	-0.8	0.8
4	100		50	50	34	5.1	0 (Process Pinch)
5	250		40	40	74	11.1	5.1
6	400	100		-100	-26	10.4	16.2
7	0 (TMP)		$\boldsymbol{F_{ifw}}$ **= 26**	26	$\boldsymbol{F_{ww}}$**= 0**		26.6

Now, to update the pre-assumed TMP concentration, associating cumulative mass load in column 8 (26.6 kg/h) is divided by the impure utility flow rate (26 to/h). The TMP contaminant concentration is calculated as 1023 ppm. The feasible WCT for scenario 3 including all the targets is listed in Table 7.10. The flow rate allocations of pinch-causing source to Higher Quality Region (HQR) and Lower Quality Region (LQR) are set as 16 ton/h and 34 ton/h, respectively. These targets can be found across the process pinch in the 6th column of Table 7.10. Furthermore, the utility pinch point is placed at the TMP concentration corresponding to zero cumulative mass load in column 8.

Table 7.10.Feasible water cascade table including all targets for scenario 3

1	2	3	4	5	6	7	8
k	C_k (ppm)	S.F_{SKj} (ton/h)	S.F_{SRi} (ton/h)	S.F_{SRi}- S.F_{SKj} (ton/h)	$F_{c,k}$ (ton/h)	Δm_k (kg/h)	Cum. Δm_k (kg/h)
1	0				$\boldsymbol{F_{fw}}$**= 34**	0.68	
2	20	50	20	-30	4	0.12	0.68
3	50	20		-20	$\boldsymbol{F_{HQR}}$= -16	-0.8	0.8
4	100		50	50	$\boldsymbol{F_{LQR}}$ =34	5.1	0 (Process Pinch)
5	250		40	40	74	11.1	5.1
6	400	100		-100	-26	-16.2	16.2
7	1023 (TMP)		$\boldsymbol{F_{ifw}}$ **= 26**	26	$\boldsymbol{F_{ww}}$**= 0**		0 (Utility Pinch)

Employing NNA method, the water allocation network is depicted in Figure 7.13.

		F_{SKj} (ton/h)	50	20	100
		C_{SKj} (ppm)	20	50	400
F_{SRi} (ton/h)	C_{SRi} (ppm)	SKj / SRi	SK1	SK2	SK3
34	**0**	**FW**	24	10	
20	20	SR1	20		
50	100	SR2	6	10	34
40	250	SR3			40
26	**1023**	**IFW**			26

Figure 7.13.Network design for scenario 3

All the targets are achieved through the network design. 16 ton/h of SR2 (pinch-causing source) is utilised for SK1& SK2 located in higher quality region and the remaining flow rate is reused to SK3 located in lower quality region. More interestingly, the introduction of impure freshwater utility with the TMP concentration for the third scenario not only satisfies the flow rate demand of lowest quality process sink (SK3) but also fulfils SK3's mass load requirement. This fact does not occur for the other threshold problems discussed in this chapter and Chapter 4. Usually, the mass load of lowest quality process sink is not entirely picked up by the available sources in the threshold problems.

7.4 Summary

This chapter presents the three categories of the "threshold problems" in the water network synthesis, including: zero network discharge with fresh water feed, network generated waste without fresh water feed, and network with no fresh water feed and no waste discharge. To highlight the contribution of this study, some important findings are as follows:

- Applying the tree steps procedure of general WCA (Foo, 2007) outlined in Chapter 3 is not applicable for targeting impure utility above the ITPP. After the flow rate adjustment for the lower quality water source, the shortage of flow rate (negative value) will occur. This shows the importance of the ITPP concentration target prior to harvesting external utility.
- The flow rate target for any utility with concentration higher than the ITPP or lower than the TMP concentration is identical and equals the absolute of infeasible (negative) waste water flow rate, which cannot be located correctly through the traditional WCA approach. These arguments justify the necessity of our proposed adjustment in WCA targeting method for targeting the flow rate of external utility in the "threshold problem without waste discharge".
- The heuristics proposed by Alwi and Manan (2007) for targeting multiple utilities flow rates using MRPD technique described in Chapter 3 is also not appropriate in scenario 3. To apply this method, it should be preliminary identified if the impure utility is below or

above the ITPP concentration. The general MRPD approach (El-Halwagi et al., 2003; Prakash and Shenoy, 2005b) can locate the flow rate target for the impure utility (the absolute value of negative waste water flow rate) in this scenario; however, its concentration should be checked to be lower than the TMP concentration.

In conclusion, taking consideration of higher quality impure water source provides more room for pure fresh water saving.

8. CONCLUSIONS AND RECOMMENDATIONS

Water scarcity is affecting many people worldwide. Furthermore, this matter gets worse in time since the amount of freshwater usage has been increasing rapidly. One of the huge consumers of freshwater is industrial processes. Thus, there is a great potential of water saving in such industries. A framework for addressing water saving opportunities in process industries has been proposed in this study using process integration approach (specifically WPA as a tool). Within this framework, reuse/recycle and regeneration-reuse/recycle schemes are considered. Moreover, a special attention has been given to the threshold problems.

From a systematic literature review, the chronological development of water pinch targeting methods has been identified. Analysis of various water pinch methodologies revealed several issues worthy of further investigation:

- For regeneration-reuse/recycle scheme, a hybrid targeting method which can address all the key parameters in total water regeneration system has not been reported. Moreover, not much attention has been paid for targeting Removal Ratio type regeneration unit and economic aspect of total water regeneration system.
- Threshold problem without waste discharge is the specific problem of reuse/recycle network. Impure utilities harvesting is the only water saving solution for this case which has lagged behind in the literature.

This research has aimed at addressing these gaps:

1) Application of Composite Table Algorithm for various problems in reuse/recycle water network

Since the introduction of WPA, many targeting methodologies have been developed and extended for various problems. It was found that CTA has several advantageous over other targeting methods:

- It is a unique graphical and numerical targeting method. Thus, it can provide both numerical accuracy and conceptual insight at the same time.
- It is more aligned with the early work of WPA i.e. the LCC. Therefore, it has a good potential to be extended for diverse water network problems;
- It requires less calculation effort.

The applicability of CTA for some other problems in reuse/recycle network including FL, hybrid FL and FF, multiple pinches, and threshold problems have been explored. As a result, it can be argued that CTA is also one of the well-established targeting approaches and is even superior to other methods due to the above-mentioned advantages.

2) Total regeneration water network optimization: fixed post-regeneration concentration

Extended Composite Table Algorithm (ECTA) has been proposed for targeting total water regeneration network. This method can set all key parameters in regeneration network comprising freshwater, regenerated, and wastewater flow rates together with regeneration and waste water concentrations with the known post-regeneration concentration. Moreover, the capability of ECTA for handling both FL and FF problems has been examined. It is demonstrated that the proposed ECTA can handle global water operation for generic problems (without the restriction of limiting composite curve shape) in a hybrid manner (both algebraically and graphically) without requiring iterative procedure. These capabilities of ECTA are exclusive compared to the available targeting methods in regeneration problems.

3) Total regeneration water network optimization: relaxed post-regeneration concentration

The assumption of specified post-regeneration concentration has been further relaxed and a new method named Composite Matrix Algorithm (CMA) was developed. By using CMA:

- A feasible region for the problem under consideration can be easily set.
- Removal Ratio (RR) graphs (RR vs. flow rate & RR vs. concentrations) can be derived to target key parameters in regeneration system when RR type regenerator is involved.
- The feasible minimum performance of regeneration unit is identified.
- The transient post regeneration concentrations causing pinch point migration can be targeted.
- The trade-off between key parameters of regeneration system is studied.
- With setting up the cost functions, the economic optimum scenario is able to be proposed.

4) Water utilities minimization for the threshold problem without waste discharge

There has been a potential for pure freshwater saving in the "threshold problem without waste discharge" via impure utility harvesting. For systematically addressing this issue, the concepts of Infeasible Threshold Problem and Infeasible Threshold Pinch Point (ITPP) have been introduced. Three different scenarios have been proposed for targeting impure utility and recovering the problem feasibility.

(1) Employment more pure fresh water source;
(2) Harvesting of the impure utility with the concentration lower than ITPP
(3) Use of the impure water source higher than ITPP

Under the second scenario, two case studies revealed that the higher quality impure utility leads to the more pure freshwater saving while keeping the total utility requirement unchanged. For the third scenario, the new target termed as Threshold Maximum Permissible (TMP) concentration has been proposed. It was concluded that, in order to utilise the impure utility above the ITPP, its quality (concentration) should be checked to be lower than TMP concentration. Moreover, this study discovered that the general WCA method requires some adjustment to be applicable for utilities targeting in "threshold problem without waste discharge".

Despite all the above achievements and contributions, future research can be recommended in several aspects as identified below:

a) ECTA and CMA methods have been developed for total regeneration water system where freshwater and regenerated water flow rates are considered to be identical. In some cases, the freshwater flow rate can be higher (partial regeneration) or lower (regeneration-recycle) than the regenerated water flow rate because of mass load infeasibility occurrence. Moreover, zero waste disposal network can be only achievable under regeneration-recycle water network. The developed ECTA and CMA can be improved to be applicable for partial regeneration, regeneration-recycle, and zero waste disposal.
b) In this study, cost evaluation was considered under the assumption of fixed unit costs. Varying unit cost will lead to a different water network. For instance, the total water regeneration network has an economic justification over the maximum reuse/recycle system when the regeneration cost is relatively lower than freshwater supply cost and waste disposal charge. To improve the cost optimization of the total water regeneration system, cost sensitivity analysis may be considered in future.
c) In utilities targeting for threshold problem without waste discharge, it was assumed that the impure utility is virtually free of cost compared to pure freshwater source. Taking the economic aspects into account, the final targeting results may change. Economic evaluation of this special problem will improve the practicability of the current study.
d) The water network in process industries mainly consists of three parts: pre-treatment, water using, and effluent treatment. While the interaction between water using processes and effluent treatment

system is called Total Water Network (TWN) problem, the inclusion of pre-treatment system into TWN is termed as Complete Water Network (CWN). The development of ECTA and CMA for TWN and CWN can be further addressed.

e) Water regenerators are further classified as single pass and partitioning units. In single pass type, the feed water and regenerated water have the same flow rate, while in the latter type the flow rate of purified stream is significantly lower than feed stream. ECTA and CMA are developed for the single pass regeneration unit. The enhancement of these methods for partitioning water regenerator would be valuable.

REFERENCES

Agrawal, V., Shenoy, U.V., 2006. Unified conceptual approach to targeting and design of water and hydrogen networks. AIChE Journal 52, 1071-1082.

Agrawal, V., Shenoy, U.V., 2007. Letter to the Editor. AIChE Journal 53, 3017-3017.

Almutlaq, A.M., El-Halwagi, M.M., 2007. An algebraic targeting approach to resource conservation via material recycle/reuse. International Journal of Environment and Pollution 29, 4-18.

Alves, J.J., Towler, G.P., 2002. Analysis of refinery hydrogen distribution systems. Industrial and Engineering Chemistry Research 41, 5759-5769.

Alwi, S.R.W., Manan, Z.A., 2007. Targeting multiple water utilities using composite curves. Industrial and Engineering Chemistry Research 46, 5968-5976.

Alwi, S.R.W., Manan, Z.A., 2008. Generic graphical technique for simultaneous targeting and design of water networks. Industrial and Engineering Chemistry Research 47, 2762-2777.

Aly, S., Abeer, S., Awad, M., 2005. A new systematic approach for water network design. Clean Technologies and Environmental Policy 7, 154-161.

Ataei, A., Tahouni, N., Haji Seyedi, S.M., Hashemian, S.M., Yoo, C., Panjeshahi, M.H., 2014. A Novel Approach to Hot Oil System Design for Energy Conservation. Applied Thermal Engineering.

Bagajewicz, M., 2000. A review of recent design procedures for water networks in refineries and process plants. Computers and Chemical Engineering 24, 2093-2113.

Bai, J., Feng, X., Deng, C., 2007. Graphically based optimization of single-contaminant regeneration reuse water systems. Chemical Engineering Research and Design 85, 1178-1187.

Bai, J., Feng, X., Deng, C., 2010. Optimal design of single-contaminant regeneration reuse water networks with process decomposition. AIChE Journal 56, 915-929.

Bandyopadhyay, S., Cormos, C.C., 2008. Water management in process industries incorporating regeneration and recycle through a single treatment unit. Industrial and Engineering Chemistry Research 47, 1111-1119.

Bandyopadhyay, S., Ghanekar, M.D., Pillai, H.K., 2006. Process water management. Industrial and Engineering Chemistry Research 45, 5287-5297.

Brouckaert, C., Buckley, C., 2000. Water pinch analysis: a strategic tool for water management in the food processing industry. Re-use of Process Water in the Food and Beverage Industries 17.

Cao, D., Feng, X., Duan, X., 2004. Design of water network with internal mains for multi-contaminant wastewater regeneration recycle. Chemical Engineering Research and Design 82, 1331-1336.

Castro, P., Matos, H., Fernandes, M., Pedro Nunes, C., 1999. Improvements for mass-exchange networks design. Chemical Engineering Science 54, 1649-1665.

CSIRO, Water shows its worth.

Deng, C., Feng, X., 2009. Optimal water network with zero wastewater discharge in an alumina plant, Proceedings of the 4th IASME/WSEAS international conference on Energy & environment. World Scientific and Engineering Academy and Society (WSEAS), pp. 109-114.

Deng, C., Feng, X., 2011. Targeting for conventional and property-based water network with multiple resources. Industrial and Engineering Chemistry Research 50, 3722-3737.

Deng, C., Feng, X., Bai, J., 2008. Graphically based analysis of water system with zero liquid discharge. Chemical Engineering Research and Design 86, 165-171.

Dhole, V.R., Ramchandani, N., Tainsh, R.A., Wasilewski, M., 1996. Make your process water pay for itself. Chemical Engineering 103.

Douglas, J.M., 1985. A hierarchical decision procedure for process synthesis. AIChE Journal 31, 353-362.

Douglas, J.M., 1992. Process synthesis for waste minimization. Industrial and Engineering Chemistry Research 31, 238-243.

Dunn, R.F., El-Halwagi, M.M., 2003. Process integration technology review: background and applications in the chemical process industry. Journal of Chemical Technology and Biotechnology 78, 1011-1021.

El-Halwagi, M.M., 1997. Pollution prevention through process integration: systematic design tools. Academic Press, San Diego.

El-Halwagi, M.M., 2006. Process integration. Academic Press, Amsterdam.

El-Halwagi, M.M., 2011. Sustainable design through process integration. Butterworth-Heinemann, Amsterdam.

El-Halwagi, M.M., Gabriel, F., Harell, D., 2003. Rigorous graphical targeting for resource conservation via material recycle/reuse networks. Industrial and Engineering Chemistry Research 42, 4319-4328.

El-Halwagi, M.M., Manousiouthakis, V., 1989. Synthesis of mass exchange networks. AIChE Journal 35, 1233-1244.

Feng, X., Bai, J., Zheng, X., 2007. On the use of graphical method to determine the targets of single-contaminant regeneration recycling water systems. Chemical Engineering Science 62, 2127-2138.

Feng, X., Chu, K.H., 2004. Cost optimization of industrial wastewater reuse systems. Process Safety and Environmental Protection 82, 249-255.

Foo, D.C.Y., 2007. Water cascade analysis for single and multiple impure fresh water feed. Chemical Engineering Research and Design 85, 1169-1177.

Foo, D.C.Y., 2008. Flowrate targeting for threshold problems and plant-wide integration for water network synthesis. Journal of Environmental Management 88, 253-274.

Foo, D.C.Y., 2009. State-of-the-art review of pinch analysis techniques for water network synthesis. Industrial and Engineering Chemistry Research 48, 5125-5159.

Foo, D.C.Y., 2012. Process integration for resource conservation. CRC Press, Boca Raton.

Foo, D.C.Y., El-Halwagi, M.M., Tan, R.R., 2012. Recent advances in sustainable process design and optimization. World Scientific.

Foo, D.C.Y., Manan, Z.A., Tan, Y.L., 2006. Use cascade analysis to optimize water network Chemical Engineering Progress 102, 45-52.

Foo, D.C.Y., Tan, R.R., Ng, D.K.S., 2008. Carbon and footprint-constrained energy planning using cascade analysis technique. Energy 33, 1480-1488.

Gomes, J.F.S., Queiroz, E.M., Pessoa, F.L.P., 2007. Design procedure for water/wastewater minimization: single contaminant. Journal of Cleaner Production 15, 474-485.

Gouws, J.F., Majozi, T., Foo, D.C.Y., Chen, C.-L., Lee, J.-Y., 2010. Water minimization techniques for batch processes. Industrial and Engineering Chemistry Research 49, 8877-8893.

Gundepsen, T., Naess, L., 1988. The synthesis of cost optimal heat exchanger networks:: An industrial review of the state of the art. Computers and Chemical Engineering 12, 503-530.

Hall, S., 1997. Water and effluent minimisation, Symposium papers-institution of chemical engineers north western branch. Institution of chemical engineers north western branch, pp. 8-8.

Hallale, N., 2002. A new graphical targeting method for water minimisation. Advances in Environmental Research 6, 377-390.

Hlaváček, V., 1978. Synthesis in the design of chemical processes. Computers and Chemical Engineering 2, 67-75.

Hohmann, E.C., 1986. Optimum networks for heat exchange. UMI.

Jacob, J., Kaipe, H., Couderc, F., Paris, J., 2002. Water network analysis in pulp and paper processes by pinch and linear programming techniques. Chemical Engineering Communications 189, 184-206.

Jeżowski, J., 2010. Review of water network design methods with literature annotations. Industrial and Engineering Chemistry Research 49, 4475-4516.

Johns, W., 2001. Process Synthesis: Poised for a wider role. Chemical Engineering Progress 97, 59-59.

Kemp, I.C., 2007. Pinch analysis and process integration: a user guide on process integration for the efficient use of energy. Butterworth Heinemann, Amsterdam.

Kim, J.K., 2012. System analysis of total water systems for water minimization. Chemical Engineering Journal 193, 304-317.

Kim, J.K., Smith, R., 2001. Cooling water system design. Chemical Engineering Science 56, 3641-3658.

Klemes, J., 2013. Handbook of Process Integration (PI): Minimisation of energy and water use, waste and emissions. Elsevier.

Klemes, J., Friedler, F., Bulatov, I., Varbanov, P., 2010. Sustainability in the process industry: integration and optimization. McGraw Hill, New York.

Kuo, W.C.J., Smith, R., 1997. Effluent treatment system design. Chemical Engineering Science 52, 4273-4290.

Kuo, W.C.J., Smith, R., 1998a. Design of water-using systems involving regeneration. Process Safety and Environmental Protection 76, 94-114.

Kuo, W.C.J., Smith, R., 1998b. Designing for the interactions between water-use and effluent treatment. Chemical Engineering Research and Design 76, 287-301.

Li, X., Kraslawski, A., 2004. Conceptual process synthesis: past and current trends. Chemical Engineering and Processing: Process Intensification 43, 583-594.

Liao, Z., Wang, J., Yang, Y., 2007. Letter to the editor. AIChE Journal 53, 1898-1899.

Linnhoff, B., Engineers, I.o.C., 1982. User guide on process integration for the efficient use of energy. Pergamon Press Oxford, UK.

Linnhoff, B., Flower, J.R., 1978. Synthesis of heat exchanger networks: I. Systematic generation of energy optimal networks. AIChE Journal 24, 633-642.

Liu, Y., Yuan, X., Luo, Y., 2007. Synthesis of water utilization system using concentration interval analysis method (I) Non-mass-transfer-based operation. Chinese Journal of Chemical Engineering 15, 361-368.

Manan, Z.A., Alwi, S.R.W., Ujang, Z., 2006. Water pinch analysis for an urban system: a case study on the Sultan Ismail Mosque at the Universiti Teknologi Malaysia (UTM). Desalination 194, 52-68.

Manan, Z.A., Tan, Y.L., Foo, D.C.Y., 2004. Targeting the minimum water flow rate using water cascade analysis technique. AIChE Journal 50, 3169-3183.

Mann, J.G., Liu, Y.A., 1999. Industrial water reuse and wastewater minimization. McGraw Hill, New York.

Manousiouthakis, V., Allen, D., 1995. Process synthesis for waste minimization. New York, NY: American Institute of Chemical Engineers, 1971-c2002., pp. 72-86.

News, B., 22 March 2002. UN warns of looming water crisis.

Ng, D.K.S., Foo, D.C.Y., 2006. Evolution of water network using improved source shift algorithm and water path analysis. Industrial and Engineering Chemistry Research 45, 8095-8104.

Ng, D.K.S., Foo, D.C.Y., Tan, R.R., 2007a. Targeting for total water network. 2. Waste treatment targeting and interactions with water system elements. Industrial and Engineering Chemistry Research 46, 9114-9125.

Ng, D.K.S., Foo, D.C.Y., Tan, R.R., Pau, C.H., Tan, Y.L., 2009. Automated targeting for conventional and bilateral property-based resource conservation network. Chemical Engineering Journal 149, 87-101.

Ng, D.K.S., Foo, D.C.Y., Tan, R.R., Tan, Y.L., 2007b. Ultimate flowrate targeting with regeneration placement. Chemical Engineering Research and Design 85, 1253-1267.

Ng, D.K.S., Foo, D.C.Y., Tan, R.R., Tan, Y.L., 2008. Extension of targeting procedure for “Ultimate flowrate targeting with regeneration placement” by Ng et al., Chem. Eng. Res. Des., 85 (A9): 1253–1267. Chemical Engineering Research and Design 86, 1182-1186.

Nishida, N., Stephanopoulos, G., Westerberg, A., 1981. A review of process synthesis. AIChE Journal 27, 321-351.

Olesen, S., Polley, G., 1997. A simple methodology for the design of water networks handling single contaminants. Chemical Engineering Research and Design 75, 420-426.

Panjeshahi, M.H., Ataei, A., Gharaie, M., Parand, R., 2009. Optimum design of cooling water systems for energy and water conservation. Chemical Engineering Research and Design 87, 200-209.

Polley, G.T., Polley, H.L., 2000. Design better water networks. Chemical Engineering Progress 96, 47-52.

Prakash, R., Shenoy, U.V., 2005a. Design and evolution of water networks by source shifts. Chemical Engineering Science 60, 2089-2093.

Prakash, R., Shenoy, U.V., 2005b. Targeting and design of water networks for fixed flowrate and fixed contaminant load operations. Chemical Engineering Science 60, 255-268.

Rudd, D.F., 1968. The synthesis of system designs: I. Elementary decomposition theory. AIChE Journal 14, 343-349.

Rudd, D.F., Powers, G.J., Siirola, J.J., 1973. Process synthesis. Prentice-Hall Englewood Cliffs, NJ.

Shenoy, U.V., 2012. Enhanced nearest neighbors algorithm for design of water networks. Chemical Engineering Science, 197-206.

Shenoy, U.V., Bandyopadhyay, S., 2007. Targeting for multiple resources. Industrial and Engineering Chemistry Research 46, 3698-3708.

Smith, R., 2005. Chemical process design and integration. Wiley New York.

Sorin, M., Bédard, S., 1999. The global pinch point in water reuse networks. Process Safety and Environmental Protection 77, 305-308.

Takama, N., Kuriyama, T., Shiroko, K., Umeda, T., 1980. Optimal water allocation in a petroleum refinery. Computers and Chemical Engineering 4, 251-258.

Tan, R.R., Ng, D.K.S., Foo, D.C.Y., 2009. Pinch analysis approach to carbon-constrained planning for sustainable power generation. Journal of Cleaner Production 17, 940-944.

Tan, Y.L., Manan, Z.A., Foo, D.C.Y., 2007. Retrofit of water network with regeneration using water pinch analysis. Process Safety and Environmental Protection 85, 305-317.

Tripathi, P., 1996. Pinch technology reduces wastewater. Chemical Engineering 103, 87-90.

Wang, Y.P., Smith, R., 1994a. Design of distributed effluent treatment systems. Chemical Engineering Science 49, 3127-3145.

Wang, Y.P., Smith, R., 1994b. Wastewater minimisation. Chemical Engineering Science 49, 981-1006.

Wang, Y.P., Smith, R., 1995. Wastewater minimization with flowrate constraints. Chemical Engineering Research and Design 73, 889-904.

Westerberg, A.W., 1987. Process synthesis: A morphological view. Recent Developments in Chemical Process and Plant Design, 127-145.

Xu, D.L., Yang, Y., Liu, Z.Y., 2013. Predicting target values of the water-using networks involving regeneration recycling. Chemical Engineering Science 104, 525-539.